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FORWARD MONTE CARLO METHOD
FOR THE SOLUTION OF
TIME-DEPENDENT HEAT CONDUCTION EQUATION

by

Eugene S. Troubetzkoy

Final Report

to

U. S. Army Research Office

Contract No. DAAG29-76-C-0035

Mathematical Applications Group, Inc.
3 Westchester Plaza
Elmsford, New York 10523

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) A forward Monte Carlo method has been developed to solve the time-dependent heat conduction or diffusion equation. The general method has been implemented so as to cover a variety of boundary conditions. The method is based on a "floating volume" random walk, similar to the one in an adjoint method. A novel problem has been posed, and successfully solved, on the treatment of boundary conditions. The solution required the introduction of a biasing function, leading to a biased random walk. The first step of the random walk is particular to the forward method. The succeeding steps can be considered self-adjoint, → over

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20. ABSTRACT CONTINUED

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TABLE OF CONTENTS

I. INTRODUCTION

A forward Monte Carlo method has been developed to solve the time-dependent heat conduction or diffusion equation. The general method has been implemented so as to cover a variety of boundary conditions.

The method is based on a "floating volume" random walk, similar to the one in an adjoint method[1]. A novel problem has been posed, and successfully solved, on the treatment of boundary conditions. The solution requires the introduction of a biasing function, leading to a biased random walk. The first step of the random walk is particular to the forward method. The succeeding steps can be considered self-adjoint, as they are identical in the forward and adjoint case. It is hoped that our study of biased random walks will also prove useful in any future development of importance biased adjoint methods.

The detailed analysis and computer implementation are still under way. The details of sampling algorithms have been completely worked out in the case of known temperature boundary conditions. Sections VIII.2 through IX.2.2, as well as Appendix B, are confined to this type of boundary condition. The remainder of the report, including Appendix A, applies to general "radiation type" boundary conditions.

II. DERIVATION OF AN INTEGRAL EQUATION

Let us consider the heat conduction equation*

$$D\nabla_x^2 T(x,t) - \frac{\partial T(x,t)}{\partial t} = 0 \qquad (1)$$

defined over a volume Ω_1 enclosed on a surface Σ_1, with the initial conditions

$$T(x,0) \text{ given for } x\varepsilon\Omega_1 \qquad (2)$$

and the boundary condition

$$\left.\begin{aligned} &\alpha(x)\,\frac{\partial T(x,t)}{\partial n} = T_g(x,t) - T(x,t) && x\varepsilon\Sigma_1 \\ &T_g(x,t) \text{ given} && 0\leq t\leq t_0 \end{aligned}\right\} \qquad (3)$$

The problem is to estimate the temperature profile at a given time t_0. For that purpose, it will be useful to introduce three Green's functions G_i, i=0, 1,2 satisfying the following equation:

$$D\,\nabla_x^2\, G_i(x,x',t_0-t) + \frac{\partial}{\partial t} G_i(x,x',t_0-t) = 0, \quad x\varepsilon\Omega_i \qquad (4)$$

with the initial condition

$$G_i(x,x',0) = \delta(x-x') \qquad x',x\varepsilon\Omega_i \qquad (5)$$

and the boundary condition

$$\begin{aligned} &G_i(x,x',t_0-t) = -\,\alpha(x)\,\frac{\partial}{\partial n} G_i(x,x',t_0-t) && x',x\varepsilon\Omega_i \\ &\alpha(x) \geq 0 && 0\leq t\leq t_0 \end{aligned} \qquad (6)$$

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*For simplicity of discussion, we assume that the diffusion coefficient D=K/ρc is constant. The method is readily generalized to the case of D=constant in finite geometrical regions, with discontinuous variation of K, ρ, and c across boundaries.

Multiplying Equation (1) by $G_1(x,x',t_0-t)$, Equation (4), written for i=1, by $T(x,t)$, subtracting and integrating over Ω, and over time, we obtain, after applying Green's theorem

$$\int_0^{t_0} dt \int_{\Sigma_1} \left[G_1(x,x',t_0-t)\, D \frac{\partial}{\partial n} T(x,t) - T(x,t)\, D \frac{\partial}{\partial n} G_1(x,x',t_0-t) \right] dS_x$$

$$- \int_0^{t_0} dt \int_{\Omega_1} \left[G_1(x,x',t_0-t) \frac{\partial}{\partial t} T(x,t) + T(x,t) \frac{\partial}{\partial t} G_1(x,x',t_0-t) \right] dV_x$$

Taking into account the boundary conditions (3) and (6) is the surface term, and the initial conditions (2) and (5) in the volume term, we obtain:

$$\int_0^{t_0} dt \int_{\Sigma_1} T_g(x,t)\, D \frac{-\partial}{\partial n} G_1(x,x',t_0-t)\, dS_x$$

$$+ \int_{\Omega_1} G_1(x,x',t_0) T(x,0)\, dV_x - T(x',t_0) = 0$$

or, interchanging x and x':

$$T(x,t_0) = V(x) + S(x) \tag{7}$$

where

$$V(x) = \int_{\Omega_1} T(x',0)\ G_1\ (x',x,t_0)\, dV_{x'} \tag{8}$$

$$S(x) = \int_0^{t_0} dt \int_{\Sigma_1} D\ T_g(x',t_0-t) \frac{-\partial}{\partial n'} G_1(x',x,t)\, dS_{x'} \tag{9}$$

The object of forward Monte Carlo is to generate a population of weighted points $x \epsilon \Omega_1$ with a density $T(x,t_0)$ for given t_0.

III. INTRODUCTORY MONTE CARLO ALGORITHM

A simple and correct Monte Carlo approach to this problem is to consider Equation (7) as the sum of two terms to be sampled separately.

The volume terms Equation (8) presents no difficulty. One can sample x' from a probability distribution function (pdf) proportional to T(x',0). Given x' and t_0, one can sample x from G_1 (x',x,t_0) using the self-adjoint method developed previously.

The surface term Equation (9) is not as straight forward to handle. The kernel $\frac{-\partial}{\partial n'} G_1(x',x,t)$ cannot be reduced to a pdf because

$$\int_{\Omega_1} \frac{-\partial}{\partial n'} G_1(x',x,t)\, dV_x \underset{t\to 0}{\longrightarrow} \infty .$$

Let us, however, define a function $G_2(x,x',t)$ which satisfies Equations (4-6) for i=2, and the function

$$Q(x',t) = \int_{\Omega_2} \frac{-\partial}{\partial n'} G_2(x',x,t)\, dV_x \tag{10}$$

It is shown in Appendix A that if the surfaces Σ_1 and Σ_2 has the same outward normal at x' (see Figure 1), then

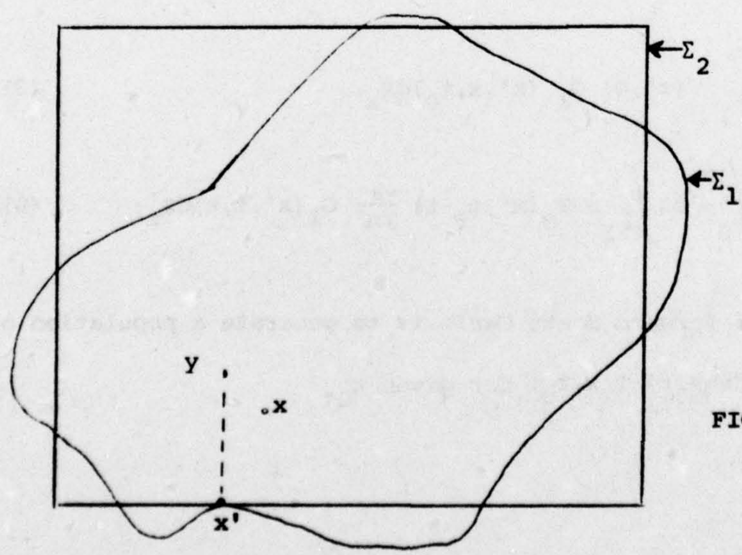


FIGURE 1

$$\int_{\Omega_1} - \frac{\partial}{\partial n'} G_1(x',x,t)dV_x \;/\; Q(x',t) \quad < \infty \quad \text{for all } t \geq 0$$

which implies that the kernel

$$- \frac{\partial}{\partial n'} G_1(x',x,t) \;/\; Q(x',t) \tag{11}$$

can be reduced to a pdf in x.

The surface term can be rewritten in the form

$$S(x) = \int_0^{t_0} dt \int_{\Sigma_1} \left[DT_g(x',t_0-t)Q(x',t) \right] \left[\frac{-\frac{\partial}{\partial n'} G_1(x',x,t)}{Q(x',t)} \right] dS_{x'} \tag{12}$$

To sample that term, one can first sample $x' \varepsilon \Sigma_1$ and t, $0<t<t_0$, from a pdf proportional to

$$T_g(x',t_0-t)Q(x',t)$$

and, given x' and t, sample x from a pdf proportional to the kernel (11).

The function Q(x',t) can be considered as a biasing, or importance function. It is defined (Equations 10 and 4) over a "floating importance volume" Ω_2, which we define more precisely as $\Omega_2^{x'}$, the superscript x' expressing the fact that the surface $\Sigma_2^{x'}$ is tangent to Σ_1 at x'. The shape of $\Omega_2^{x'}$ is otherwise arbitrary; it can be chosen simply enough such that Q be analytically known. In practice, we will eventually restrict the surface $\Sigma_2^{x'}$ to be an infinite plane tangent to Σ_1 at x'.

As long as we have the necessity to introduce a biasing function for sampling the surface term (9), we find it also desirable to introduce a biasing function for the volume term (8). In order to define such a function, let us first generalize the definition of "floating importance volume". The floating volume $\Omega_2^{x'}$ has been defined for points x' on Σ_1. Let us now consider a point y internal to the configuration. Let x' be the point on Σ_1 closest to y (see

Figure 1). We define the "floating importance volume" associated with y as any volume Ω_2, its surface Σ_2 being tangent to Σ_1 at x'. We generalize our definition of superscripts and denote that volume as Ω_2^y. The restricted definition of the last paragraph is preserved as y and x' coincide if y approaches the surface Σ_1. Let us now define the function

$$E_y(z,t) = \int_{\Omega_2^y} G_2(z,x,t)\,dV_x \qquad (13)$$

where $G_2(z,x,t)$ satisfies Equations (4-6) for i=2 and $\Omega_2 \equiv \Omega_2^y$.

We propose to use Eq. $E_y(x,t)$ as a biasing function for internal points y, and rewrite the volume term (8) in the form

$$V(x) = \int_{\Omega_1} \left[T(x',0)\; E_{x'}(x',t_0) \right] \frac{G_1(x',x,t_0)}{E_{x'}(x',t_0)}\, dV_{x'} \qquad (14)$$

IV. A PRACTICAL MONTE CARLO ALGORITHM

Equation (14) can be rewritten as

$$V(x) = T_V U_V(x) \tag{15}$$

where

$$T_V = \int_{\Omega_1} T(x',0) E_x(x',t_0) dV_{x'} \tag{16}$$

and

$$U_V(x) = \int_{\Omega_1} p_V{}^0(x') \frac{G_1(x',x,t_0)}{E_{x'}(x',t_0)} dV_{x'} \tag{17}$$

$$p_V{}^0(x') = T(x',0) E_{x'}(x',t_0)/T_V \tag{18}$$

Similarly, Equation (12) can be rewritten as

$$S(x) = T_S U_S(x) \tag{19}$$

where

$$T_S = \int_0^{t_0} dt \int_{\Sigma_1} DT_g(x',t_0-t) Q(x',t)\ dS_{x'} \tag{20}$$

$$U_S(x) = \int_0^{t_0} dt \int_{\Sigma_1} p_S{}^0(x',t) \frac{-\frac{\partial}{\partial n'} G_1(x',x,t)}{Q(x',t)} dS_{x'} \tag{21}$$

$$p_S{}^0(x',t) = DT_g(x',t_0-t) Q(x',t)/T_S \tag{22}$$

Substituting (15) and (19) into (7), we obtain

$$T(x,t_0) = T_T U_T(x) \tag{23}$$

where

$$T_T = T_V + T_S \tag{24}$$

and

$$U_T(x) = P_V U_V(x) + (1-P_V) U_S(x) \tag{25}$$

$$P_V = T_V/T_T \tag{26}$$

As stated previously, the object of a forward Monte Carlo method is to generate a population of weighted points representing the density $T(x,t_0)$ for given t_0. We define a random member of such a population as a sample of $T(x,t_0)$, and the process of generation of such a member as sampling $T(x,t_0)$.

According to Equation (23), in order to sample $T(x,t_0)$, we can sample $U_T(x)$ and multiply the weight by T_T. To sample $U_T(x)$, consider Equation (25). With probability p_V, sample $U_V(x)$, else sample $U_S(x)$.

We now turn to prescribe methods to sample $U_V(x)$ and $U_S(x)$. In the case of $U_V(x)$, consider its definition (Equation 17). To sample, we can first sample x' from the pdf $p_V{}^0(x')$ defined by Equation (18) and, given x' (and t_0), sample x from the kernel

$$K_V(x',x,t_0) = G_1(x',x,t_0)/E_x(x',t_0) \tag{27}$$

In the case of $U_S(x)$, consider its definition (Equation 21). To sample, we can first sample x' and t from the pdf $p_S{}^0(x',t)$ defined by Equation (22) and, given x' and t, sample x from the kernel

$$K_S(x',x,t) = \frac{-\partial}{\partial n'} G_1(x',x,t)/Q(x',t) \tag{28}$$

The sampling of the kernels (27) and (28) can be achieved by constructing a random walk which we are about to describe. The walks for K_V and K_S are identical except for the first step.

V. THE BIASED FLOATING VOLUME RANDOM WALK

V.1 The Integral Equation

As defined previously, the configuration under investigation is bounded by a surface Σ_1, with a volume Ω_1. We also defined a "simple" surface Σ_2, with a volume Ω_2, tangent to Σ_1 at a variable point x' (see Figure 2). In addition, let us define another "simple" surface Σ_0 with a volume Ω_0, which is wholly contained in both Ω_1 and Ω_2, and a Green's function G_0 defined over Ω_0, which satisfies Equations (4) and (6) for i=0. We rewrite these equations and write the initial conditions in the form

$$D\,\nabla_x^2\, G_0(x,x'',t) - \frac{\partial}{\partial t} G_0(x,x'',t) = 0 \qquad x\varepsilon\Omega_0 \tag{29}$$

$$G_0(x,x'',0) = \delta(x-x'') \qquad x\varepsilon\Omega_0 \tag{30}$$

$$G_0(x,x'',t) = -\,\alpha(x)\,\frac{\partial}{\partial n} G_0(x,x'',t) \qquad x\varepsilon\Omega_0 \tag{31}$$

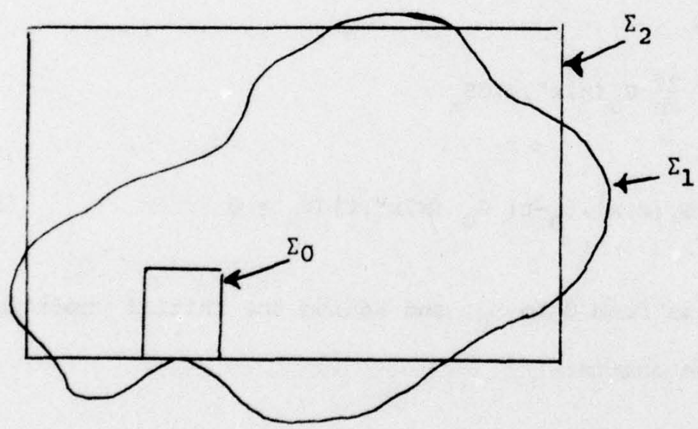


FIGURE 2.

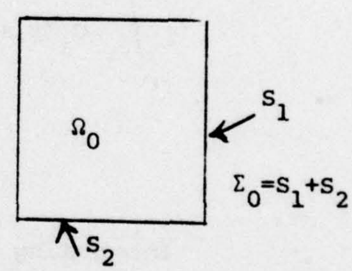


FIGURE 3.

Let $\Sigma_0 = S_1 + S_2$, where S_2 is the common part, if any, of Σ_0, Σ_1, Σ_2 and S_1 is the rest of Σ_0 which is internal to Σ_1 and Σ_2.

Let

$$\alpha_0(x) = \alpha_1(x) = \alpha_2(x) \quad \text{for } x\varepsilon S_2 \tag{32}$$

and

$$\alpha_0(x) = 0 \qquad \text{for } x\varepsilon S_1 \tag{33}$$

Multiplying Equation (4) by G_0, Equation (29) by G_i, subtracting, and integrating over Ω_0, we obtain, after applying Green's theorem:

$$\int_{\Sigma_0}\left[G_0(x,x'',t)\,\frac{\partial}{\partial n}\,G_i(x,x;,t_0-t) - G_i(x,x',t_0-t)\,\frac{\partial}{\partial n}\,G_0(x,x'',t)\right] dS_x$$

$$+\int_{\Omega_0}\left[G_0(x,x'',t)\,\frac{\partial}{\partial t}\,G_i(x,x',t_0-t)\right.$$

$$\left.+\,G_i(x,x',t_0-t)\,\frac{\partial}{\partial t}\,G_0(x,x'',t)\right] dV_x=0 \qquad (34)$$

The Σ_0 - integral can be broken up into an S_1-integral and an S_2-integral. The S_2-integral vanishes because of the boundary conditions (6), (31), and (32). The first term of the S_1-integral vanishes because of the boundary conditions (31) and (33). The integrand of the volume term can be rearranged. Equation (34) can be rewritten as

$$\int_{S_1} G_i(x,x',t_0-t)\,\frac{-\partial}{\partial n}\,G_0(x,x'',t)\,dS_x$$

$$+\,\frac{\partial}{\partial t}\int_{\Omega_0} G_i(x,x',t_0-t)\;G_0\;(x,x'',t)\,dV_x = 0 \qquad (35)$$

Integrating over time from 0 to t_0, and taking the initial conditions (5) and (30) into account, we obtain:

$$G_i(x'',x',t_0) = G_0(x',x'',t_0)$$

$$+\int_0^{t_0} dt \int_{S_1} G_i(x,x',t_0-t)\,\frac{-\partial}{\partial n}\,G_0(x,x'',t)\,dS_x \qquad (36)$$

or, dividing by $E_{x''}(x'',t_0)$ defined by Equation (13):

$$\left[\frac{G_i(x'',x',t_0)}{E_{x''}(x'',t_0)}\right] = \frac{G_0(x',x'',t_0)}{E_{x''}(x'',t_0)}$$

$$+\int_0^{t_0} dt \int_{S_1} \left[\frac{G_i(x,x',t_0-t)}{E_x(x,t_0-t)}\right]\left[\frac{E_x(x,t_0-t)}{E_{x''}(x,t_0-t)}\right] \frac{E_{x''}(x,t_0-t)\,\frac{-\partial}{\partial n}\,G_0(x,x''t)}{E_{x''}(x'',t_0)}\,dS_x \tag{37}$$

Equation (37), written for i=1, can be considered as an integral equation for $K_V(x'',x',t_0)$ defined by Equation (27).

Writing Equation (37) for i=2, integrating x' over Ω_2, and taking (13) into account, we obtain

$$1 = \int_{\Omega_0} \frac{G_0(x',x'',t_0)}{E_{x''}(x'',t_0)}\,dV_{x'} + \int_0^{t_0} dt \int_{S_1} \frac{E_{x''}(x,t_0-t)\,\frac{-\partial}{\partial n}\,G_0(x,x'',t)}{E_{x''}(x'',t_0)}\,dS_x \tag{38}$$

Similar manipulations on Equation (35) lead to the following equation which will prove very useful:

$$p(t,t_0,x'') = -\frac{\partial}{\partial t}\,F(t,t_0,x'') \tag{39}$$

where

$$p(t,t_0,x'') = \int_{S_1} \frac{E_{x''}(x,t_0-t)\,\frac{-\partial}{\partial n}\,G_0(x,x'',t)}{E_{x''}(x'',t_0)}\,dS_x \tag{40}$$

and

$$F(t,t_0,x'') = \int_{\Omega_0} \frac{E_{x''}(x,t_0-t)\,G_0(x,x'',t)}{E_{x''}(x'',t_0)}\,dV_x \tag{41}$$

Equation (32) shows that the kernel of Equation (37), except for the factor $E_x(x,t_0-t)/E_{x''}(x,t_0-t)$ in the surface term, is a normalized kernel.

The factor $E_x/E_{x''}$ is identically equal to unity if the ideal biasing function is used. The ideal biasing function is achieved if the "floating importance volume" Ω_2^y coincides with the volume of the configuration Ω_1 for all points y. The factor is expected to deviate little from unity is Ω_2^x and $\Omega_2^{x''}$ closely match Ω_1 in the neighborhood of both x and x".

An integral representation similar to Equation (37) can be derived for the kernel $K_S(x',x,t_0)$ defined by Equation (28). For that purpose, consider Equation (36) with x" on the common part of Σ_1 and Σ_2, and take the normal derivative $\partial/\partial n''$ of that equation at point x". Dividing the result by $-Q(x'',t_0)$ (defined by Equation 10), one obtains:

$$\left[\frac{-\frac{\partial}{\partial n''} G_i(x'',x',t_0)}{Q(x'',t_0)}\right] = \frac{-\frac{\partial}{\partial n''} G_0(x',x'',t_0)}{Q(x'',t_0)}$$
$$+\int_0^{t_0} dt \int_{S_1} \left[\frac{G_i(x,x',t_0-t)}{E_x(x,t_0-t)}\right]\left[\frac{E_x(x,t_0-t)}{E_{x''}(x,t_0-t)}\right] \frac{E_{x''}(x,t_0-t)\,\frac{\partial^2}{\partial n \partial n''} G_0(x,x'',t)}{Q(x'',t_0)}\, dS_x \tag{42}$$

Writing the above equation for 1=2, integrating x' over Ω_2, and taking Equation (10) into account, one obtains an equation similar to Equation (38):

$$1 = \int_{\Omega_0} \frac{-\frac{\partial}{\partial n''} G_0(x',x'',t_0)}{Q(x'',t_0)}\, dV_{x''}$$
$$+\int_0^{t_0} dt \int_{S_1} \frac{E_{x''}(x,t_0-t)\,\frac{\partial^2}{\partial n'' \partial n} G_0(x,x'',t)}{Q(x'',t_0)}\, dS_x \tag{43}$$

Equation (42) is an expression for $K_S(x'',x',t_0)$ (Equation 28) involving an integral over $K_V(x,x',t_0-t)$ (Equation 27) which, in turn, satisfies the integral Equation (27).

Finally, the equivalent of Equations (39-41) is:

$$q(t,t_0,x") = -\frac{\partial}{\partial t} H(t,t_0,x") \tag{44}$$

where

$$q(t,t_0,x") = \int_{S_1} \frac{E_{x"}(x,t_0-t)\ \frac{\partial^2}{\partial n"\partial n} G_0(x,x",t)}{Q(x",t_0)}\, dS_x \tag{45}$$

and

$$H(t,t_0,x") = \int_{\Omega_0} \frac{E_{x"}(x,t_0-t)\ \frac{-\partial}{\partial n"} G_0(x,x",t)}{Q(x",t_0)}\, dV_x \tag{46}$$

V.2 The Random Walk

V.2.1 Sampling $K_V(x",x',t_0)$

The sampling problem is the following. Given x" and t_0, sample x' from $G_1(x",x',t_0)/E_{x"}(x",t_0)$ which satisfies Equation (37). Considering the rhs of that equation, one has to sample two terms. The first term (G_0/E) can be sampled directly. To sample the second term, one can first sample t and x from the surface part of the kernel, and, given t and x, calculate the weight factor $E_x(x,t_0-t)/E_{x"}(x,t_0-t)$ and sample $G_i(x,x',t_0-t)/E_x(x,t_0-t)$. The procedure just described can be repeated for that sampling.

As shown in the previous section (Equation 38), the sum of the normalizations of the density functions of the first and second term is unity: only one of the two terms need to be sampled, with probability equal to the normalization of its kernal.

The normalization of the surface kernel is equal to:

$$1 - F(t_0,t_0,x")$$

where F is defined by Equation (39). With that probability, the time variable has to be selected from the distribution $p(t,t_0,x")$ given by Equation 39 or 40. Once t has been selected, the distribution of $x\varepsilon S_1$ is proportional to

$$r(x) \propto E_{x"}(x,t_0-t) \frac{-\partial}{\partial n} G_0(x,x",t) \tag{47}$$

with remaining probability $F(t_0,t_0,x")$, the volume term of Equation (37) is to be sampled for x'. The distribution of x' is proportional to

$$r(x') \propto G_0(x',x",t_0). \tag{48}$$

Once x' is sampled from the volume term, the random walk terminates.

V.2.2 Sampling $K_S(x",x',t_0)$

The sampling problem is quite similar to that described for K_V: given $x"$ and t_0, sample x' from $\frac{-\partial}{\partial n"} G_1(x",x',t_0)/Q(x",t_0)$ which satisfies Equation (39). The first term can be sampled directly. To sample the second term, one samples t and x from the surface part of the kernel, and given t and x, calculates the weight factor $E_x(x,t_0-t)/E_{x"}(x,t_0-t)$ and samples $K_V(x,x',t_0-t) = G_i(x,x',t_0-t)/E_x(x,t_0-t)$ by the procedure outlined in the preceding subsection.

Equation (40) shows that the sum of the normalization of the two density functions is unity: only one of the two terms need to be sampled with appropriate probability.

The probability to sample the surface kernel is equal to:

$$1 - H(t_0,t_0,x")$$

where H is defined by Equation (46). With that probability the time variable has to be sampled from the distribution $q(t,t_0,x")$ given by Equation (44) and (45). Once t has been selected, the probability distribution function of $x \varepsilon S_1$ is proportional to

$$S(x) \propto E_{x"}(x,t_0-t) \frac{\partial^2}{\partial n" \partial n} G_0(x,x",t) \tag{49}$$

With remaining probability $H(t_0,t_0,x")$, the volume term of Equation (39) has to be sampled for x'. The distribution is proportional to

$$S(x') \propto \frac{-\partial}{\partial n"} G_0(x',x",t_0) \tag{50}$$

Once x' has been sampled in this way, the random walk terminates.

VI. SPECIALIZATION TO RECTANGULAR PARALLELEPIPEDS

The derivations up to now involved completely arbitrary volumes Ω_0 and Ω_2, the only restrictions being that the surface Σ_2 surrounding Ω_2 must be tangent at a given point to the surface Σ_1 of the configuration, and that the volume Ω_0 must be internal to both Ω_1 and Ω_2. In practice, the choice of these two volumes is limited to such shapes for which the Green's functions G_0 and G_2 are known or easily computable. Carlslaw and Jaeger give Green's functions for a variety of shapes. The efficiency of the Monte Carlo technique would improve if the shapes are chosen to match, as closely as possible, the boundaries of the configuration under investigation. For simplicity, we limit the choice to rectangular parallelepipeds, the edges of Ω_1 and Ω_2 being parallel. This restriction permits an exact solution in the case of configurations with piece-wise planar boundaries, or solutions to an arbitrary degree of accuracy if curved boundaries are involved.

VI.1 Separation of Variables

We are looking for the solutions $G_i(\vec{x},\vec{x}',t)$, $i=0,2$, which satisfy Equations (4-6). Let $\vec{x}'-\vec{x} = (x_1,x_2,x_3)$ in a coordinate system parallel to the axes of the RPP. Dropping the subscript i, we are looking for the solution $G(x_1,x_2,x_3,t)$ which satisfies

$$D\left[\frac{\partial^2 G}{\partial x_1^2} + \frac{\partial^2 G}{\partial x_2^2} + \frac{\partial^2 G}{\partial x_3^2}\right] - \frac{\partial G}{\partial t} = 0 \tag{51}$$

for $a_j^- \leq x_j \leq a_j^+$, $j = 1,3$ and $t \geq 0$ with the boundary condition

$$G(x_1,x_2,x_3,t) = -\alpha_j^{\pm}\frac{\partial G(x_1,x_2,x_3,t)}{\partial x_j} \quad , x_j = a_j^{\pm} \text{ , } j = 1,3 \tag{52A}$$

where $a_j^{\pm}$, $\alpha_j^{\pm}$ are given constants:

$$\alpha_j^{\pm} = 0 \text{ for } j = 1,2, \ \alpha_3^+ = 0, \ \alpha_3^- = \alpha \tag{52B}$$

and the boundary condition

$$G(x_1,x_2,x_3,0) = \delta(x_1)\ \delta(x_2)\ \delta(x_3) \tag{53}$$

Let us assume that the solution can be written in the form:

$$G(x_1,x_2,x_3,t) = X^1(x_1,t)\ X^2(x_2,t)\ X^3(x_3,t) \tag{54}$$

Substituting (54) into (51) we obtain:

$$X^1X^2X^3 \sum_{j=1}^{3} \frac{1}{X^j}\left[D\,\frac{\partial^2 X^j}{\partial x_j^2} - \frac{\partial X^j}{\partial t}\right] = 0 \tag{55}$$

A solution of (51-53) is therefore (54) with

$$D\,\frac{\partial^2}{\partial x_j^2}\,X^j(x_j,t) - \frac{\partial}{\partial t}\,X^j(x_j,t) = 0 \tag{56}$$

$$X^j(x_j,t) = -\,\alpha_j^{\pm}\,\frac{\partial X^j(x_j,t)}{\partial x_j}\ ,\quad x_j = a_j^{\pm} \tag{57}$$

$$X^j(x_j,0) = \delta(x_j) \tag{58}$$

$j = 1,\ 2,\ 3$

The four-dimensional problem (51-54) has therefore been reduced to three two-dimensional problems (56-58).

Let us now derive the appropriate expressions for the functions E and Q defined by Equations (13) and (11), respectively.

From the definition (13):

$$E_{\vec{x}'}(\vec{x}',t) = \int_{x'_1-a^-_1}^{x'_1-a^+_1} dx_1 \int_{x'_2-a^-_2}^{x'_2-a^+_2} dx_2 \int_{x'_3-a^-_3}^{x'_3-a^+_3} dx_3 \; G\,(x'_1-x_1, x'_2-x_2, x'_3-x_3, t)$$

$$= E^1(x'_1,t)\; E^2(x'_2,t)\; E^3(x'_3,t) \tag{59}$$

where

$$E^j(x',t) = \int_{x'-a^-}^{x'-a^+_j} X^j(x'-x,t)\,dX \tag{60}$$

Let us consider $\vec{X}'$ on the surface of the configuration, the outer normal pointing in the negative X_3-direction. From the definition (11) we get:

$$Q(\vec{x}',t) = E^1(x'_1,t)\; E^2(x'_2,t)\; Q^3(x'_3,t) \tag{61}$$

where

$$Q^3(x',t) = \int_{x'-a^-_j}^{x'-a^+_j} \frac{-\partial}{\partial x'}\; X^j(x'-x,t)\,dX \tag{62}$$

VI.2 <u>Sampling the RPP Green's Functions</u>

VI.2.1 <u>For Purposes of Sampling K_V</u>

Substituting the results of the preceding subsection into Equation (41), we obtain:

$$F(t,t_0,\vec{x}'') = F^1(t,t_0,x''_1)\; F^2(t,t_0,x''_2)\; F^3(t,t_0,x''_3) \tag{63}$$

where

$$F^i(t,t_0) = \int_{x''_i-a^-_i}^{x''_i-a^+_i} \frac{E^i(x,t_0-t)\,X^i(x''_i-x,t)}{E^i(x''_i,t_0)}\,dX \tag{64}$$

Similarly, Equation (40) gives:

$$p(t,t_0,\vec{x}") = p^1F^2F^3 + F^1p^2F^3 + F^1F^2p^3 \tag{65}$$

where

$$p^i(t,t_0) = \frac{E_s^i(x_i"-a_i^-,t_0-t)\ \frac{-\partial}{\partial x}\ X^i(a_i^-,t) + E_s^i(x_i"-a_i^+,t_0-t)\ \frac{\partial}{\partial x}\ X^i(a_i^+,t)}{E^i(x_i",t_0)} \tag{66}$$

where

$$E_s^i(x,t) = E^i(x,t) \text{ if } x \neq 0$$
$$= 0 \text{ if } x = 0 \tag{66a}$$

Both F^i (Equation 64) and p^i (Equation 66) are also functions of $X_i"$.

Substituting 63 and 65 into 40, we obtain

$$p^i(t,t_0) = -\frac{\partial}{\partial t} F^i(t,t_0) \tag{67}$$

Let us recall our aim: with probability $1-F(t_0,t_0,\vec{x}")$ *sample the surface term*, i.e., first sample a time t from the distribution $p(t,t_0,\vec{x}")$. We will prove that the following algorithm will produce such a time distribution.

Perform the following for i = 1, 2, 3:

Attempt to sample t_i, $0<t_i<t_0$, from $-\frac{\partial}{\partial t_i} F^i(t_i,t_0)$. This can be done by sampling a random number ξ_i and attempting to solve $F^i(t_i,t_0) = \xi_i$ for $t_i<t_0$. The attempt will fail with probability $F^i(t_0,t_0)$, in which case set $t_i=t_0$.

When all done (t_1,t_2,t_3 sampled), set $t=\min(t_1,t_2,t_3)$.

Proof: Given any time $T\leq t_0$, the probability that the algorithm produces a time $t\geq T$ is equal to the product $F_1(T,t_0)\cdot F_2(T,t_0)\cdot F_3(T,t_0)$, which, according to Equation (63) is equal to $F(T,t_0,\vec{x}")$. The probability that $t<T$ is therefore $1-F(T,t_0,\vec{x}")$.

Setting $T=t_0$, we prove that the probability of $t<t_0$ is equal to $1-F(t_0,t_0,\vec{x}")$, as desired.

Setting T=t, we can calculate the probability distribution function of samples t delivered by the algorithm

$$\frac{\partial}{\partial t}\left[1-F(t,t_0,\vec{x}")\right]$$

which, according to Equation (39), is equal to $p(t,t_0,\vec{x}")$, as announced. The proof is thus completed.

Once $t<t_0$ has been sampled, the next step is to sample $\vec{x}$ from the distribution $r_s(\vec{x})$ given by Equation (47). Taking into account separability of variables, this can be rewritten as:

$$\begin{aligned} r_s(\vec{x}) &= r_s^1(x_1)r_v^2(x_2)r_v^3(x_3) \\ &+ r_v^1(x_1)r_s^2(x_2)r_v^3(x_3) \qquad (68) \\ &+ r_v'(x_1)r_v(x_2)r_s^3(x_3) \end{aligned}$$

where

$$r_v^i(x) = E^i(x,t_0-t)X^i(x_i"-x,t)/E^i(x_i",t_0) \qquad (69)$$

and

$$\begin{aligned} r_s^i(x) &= E_s^i(x,t_0-t)\,\frac{\partial}{\partial x}\,X^i(x_i"-x,t)\,\cdot \\ &\cdot \left[\delta(x-x_i"+a_i^-) - \delta(x-x_i"+a_i^+)\right] / E^i(x_i",t_0) \qquad (70) \end{aligned}$$

Expression (68) consists of the sum of three terms. To sample (x_1,x_2,x_3) from that expression, we can sample a single one of the three terms, with a probability proportional to that term's normalization.

Taking Equation (64) and (66) into account, we can calculate the normalization of the first term of Equation (68). It is equal to:

$$p^1(t,t_0)\;F^2(t,t_0)\;F^3(t,t_0) \qquad (71)$$

The normalization of the second and third term of (68) can be obtained from that expression by a circular permutation of the indices.

Expression (71) is equal to the probability that t_1 sampled from $p_1(t_1,t_0)$ is smaller than t_i sampled from $p_i(t_i,t_0)$ for both i=2 and 3. This property can be used to determine which of the terms of Equation (68) is to be sampled: if the time selection $t=\min(t_1,t_2 t_3)$ produced $t=t_j$ then the j^{th} term of Equation (68) is to be sampled.

To sample the j^{th} term, X_i has to be sampled from $r_v^i(x_i)$ (Equation 69), for both values of $i \neq j$. X_j is to be sampled from $r_s^j(x_j)$ (Equation 70): X_j is set equal to $x_j''-a_j^{\pm}$ with a probability proportional to

$$r_s^{j\pm} = E_s^j(x_j'' - a_j^{\pm}, t_0-t)(\pm 1)\,\frac{\partial}{\partial x}\,X^j(a_j^{\pm},t) \tag{72}$$

Finally, if the volume term of Equation (38) is to be sampled, t is set to t_0 and all x_i are to be sampled from $r_v^i(x_i)$ (Equation 69), for i=1,2,3.

The sampling of RPP Green's functions has been reduced to the sampling of one-dimensional Green's functions. This sampling will be discussed in Section VIII.

VI.2.2 <u>For Purposes of Sampling K_s</u>

Substituting the results of Section VI.1 into Equation (46), we obtain an equation similar to Equation (63):

$$H(t,t_0,x'') = F^1(t,t_0)\ F^2(t,t_0)\ H^3(t,t_0) \tag{73}$$

where $F^i(t,t_0)$ is defined by Equation (64) and

$$H^3(t,t_0) = \int_{x_3''-a_3^-}^{x_3''-a_3^+} \frac{E^3(x,t_0-t)\ \frac{-\partial}{\partial x_3''}\ X^3(x_3''-x,t)}{Q^3(x_3'',t_0)} \tag{74}$$

Similarly, Equation (45) gives an equation similar to Equation (65)

$$q(t,t_0,x'') = p^1\ F^2\ H^3 + F^1\ p^2\ H^3 + F^1\ F^2\ q^3 \tag{75}$$

where p^i is defined by Equation (66) and

$$q^3(t,t_0) = \frac{E_S^3(x''-a_i^-,t_0-t)\ \frac{\partial^2}{\partial x^2}\ X^3(a_3^-,t) + E^3(x''-a_3^+,t_0-t)\ \frac{-\partial^2}{\partial x^2}\ X^3(a_3^+,t)}{Q^3(x'',t_0)} \tag{76}$$

Substituting (73) and (75) and (67) into (40) we obtain an equation similar to Equation (67)

$$q^3(t,t_0) = -\frac{\partial}{\partial t}\ H^3(t,t_0) \tag{77}$$

As in the preceding subsection, the sampling of time can be achieved by sampling three independent times: t_1 and t_2 from p_1 and p_2, respectively, and t_3 from $q_3(t_3,t_0)$. $t=t_j=\min(t_1,t_2,t_3)$ is retained. If $t\geq t_0$, the volume term is to be sampled. Otherwise the j^{th} term of the following distribution has to be sampled:

$$r_s^i(x_1)\ r_v^2(x_2)\ S_v^3(x_3) + r_v^1(x_1)\ r_s^2(x_2)\ S_v^3(x_3) + r_v^1(x_1)\ r_v^2(x_2)\ S_s^3(x_3) \tag{78}$$

where r_v^i and r_s^i are defined by Equations (69) and (70) respectively, and

$$S_v^3(x) \propto E^3(x,t_0-t)\ \frac{\partial}{\partial x}\ X^3(x_3''-x,t)/Q^3(x_3'',t_0) \tag{79}$$

$$S_s^3(x) \propto \frac{E^3(x,t_0-t)\ \frac{-\partial^2}{\partial x^2}\ X_3(x_3''-x,t)}{Q^3(x_3'',t_0)} \left[\delta(x-x_3''+a_3^-)-\delta(x-x_3''+a_i^+)\right] \tag{80}$$

If the term

$$j = 3 \tag{81}$$

is to be sampled, the sampling of $S_s^3(x_3)$ can be achieved by setting $x_3=x_3''-a_3^{\pm}$ with a probability proportional to

$$S_s^{3\pm} = E_s^3(x_3''-a_3^{\pm},t_0-t)\ (\pm 1)\ \frac{-\partial^2}{\partial x^2}\ X^3(a_3^{\pm},t) \tag{82}$$

Finally, if the volume term of Equation (42) is to be sampled, t is set to t_0, x_i is sampled from $r_v^i(x_i)$ (Equation 69) for i=1,2, and x_3 is sampled from $S_v^3(x_3)$ (Equation 79).

The sampling of RPP Green's functions has been reduced to the sampling of one-dimensional Green's functions. This sampling will be discussed in Section VIII.

VII. FURTHER SPECIALIZATION OF THE IMPORTANCE FUNCTION

As defined by Equations (10) and (13), the importance functions $Q(\vec{x}',t)$ and $E_{\vec{x}'}(x',t)$ are defined in terms of a Green's function $G_2(\vec{x},\vec{x}',t)$, which, in turn, is defined over an RPP Ω_2 tangent to the outer surface Σ_1 of the configuration at the point of closest approach to x'. We now specialize the RPP Σ_2 to an infinite plane, as shown in Figure 4.

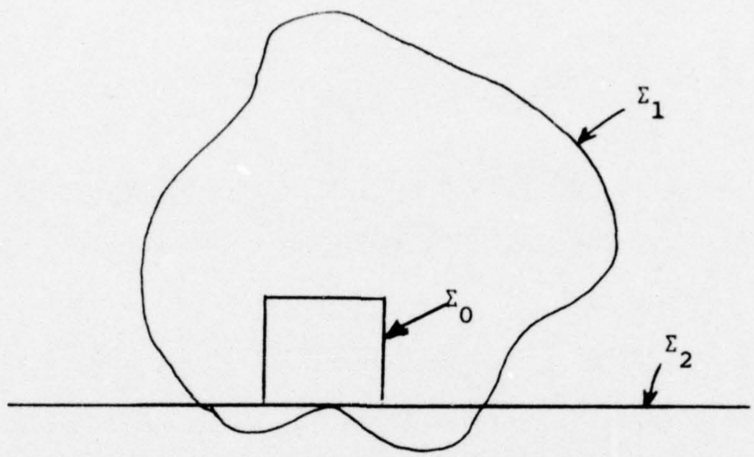


FIGURE 4

Equation (60) written for j=1,2 gives:

$$E^1(x_1',t) = E^2(x_2',t) = 1 \tag{83}$$

Equations (59) and (60) become:

$$E_{\vec{x}'}(\vec{x}',t) = E^3(x_3',t) \tag{84}$$

$$Q(\vec{x}',t) = Q^3(x_3',t) \tag{85}$$

In the following discussions, the superscript 3 of E^3 and Q^3 will be dropped.

The importance function Q is defined only if the RPP Σ_0 shares a common piece of boundary S_2 with the surface Σ_1 of the configuration. The importance function E does not have to be restricted to that case. We wish, however, to impose that restriction, and set $E^3(x_3',t) = 1$ if the RPP Σ_0 does not abut the surface Σ_1. This implies that the importance biasing will be turned off in that case.

VIII. THE ONE-DIMENSIONAL GREEN'S FUNCTIONS

The sampling of RPP Green's functions has been reduced to the sampling of one-dimensional functions defined over the solutions of one-dimensional differential equations (56). As spelled out in Section VI, the time variable has to be sampled from the p.d.f. $p^i(t,t_0)$ (Equation 66) related to the cumulative distribution $F_i(t,t_0)$ (Equation 64), or from the p.d.f. $q^3(t,t_0)$ (Equation 76) related to the cumulative distribution $H^3(t,t_0)$ (Equation 74). The spacial variables x_i have to be sampled from the p.d.f. $r_v^i(x)$ (Equation 69) or $S_v^3(x)$ (Equation 79), or from the discrete distribution $r_s^{j\pm}$ (Equation 72) or $S_s^{3\pm}$ (Equation 82). The analytical expression for all the distribution functions involved will be derived in this section. Methods to sample these distributions will be discussed in Section IX.

VIII.1 The X^1, X^2, and Related Functions

X^1 and X^2 satisfy Equations 56-58 with $\alpha_j^{\pm} = 0$. We consider the symmetric case $a_j^+ = -a_j^- = a/2$. In that case, the solutions X^1 and X^2 have been derived previously[1]. Summarizing the results, the solution can be expressed in terms of reduced variables

$$\xi = x/a \tag{86}$$

$$\tau = Dt/a^2 \tag{87}$$

$$X^i(x,t)dx = G(\xi,\tau)d\xi \tag{88}$$

and given either in the eigenfunction expansion

$$G(\xi,\tau) = 2\sum_{n=0}^{\infty} \cos\left[(2n+1)\pi\xi\right] \exp\left[-(2n+1)^2\pi^2\tau\right] \tag{89}$$

or in the image expansion

$$G(\xi,\tau) = \frac{1}{2\sqrt{\pi\tau}} \sum_{n=-\infty}^{+\infty} (-1)^n \exp\left[-(\xi+n)^2/4\tau\right] \tag{90}$$

An excellent approximation to Equation (64) with $E^i(x,t) = 1$ is given as follows:

$$F(t) = R(\tau) \tag{91a}$$

$$R(\tau) = 1 - \frac{4}{\sqrt{\pi}} \int_{1/4\sqrt{\tau}}^{\infty} e^{-u^2}\, du \quad \text{for } \tau < \tau_e \tag{91b}$$

$$R(\tau) = \frac{4}{\pi} \left[\exp(-\pi^2 \tau) - (1/3)\exp(-9\pi^2 \tau) \right] \quad \tau \geq \tau_e \tag{91c}$$

$$\tau_e = .05 \quad , \tag{91d}$$

the relative error being less than one part in ten thousand.

In terms of the reduced variables (86) and (87), Equation (67) becomes

$$p^i(\tau, \tau_0) = -\frac{d}{d\tau} R(\tau) \tag{91e}$$

Equation (69) becomes:

$$r_v^i(x)dx \propto G(\xi, \tau)d\xi \tag{92}$$

Adequate accuracy results from the use of the first two terms of Equation (89) if $\tau < .05$, and of the expansion (90) if $\tau \geq .05$.

Finally, expression (72) becomes:

$$r_s^{j\pm} = 1/2 \tag{93}$$

meaning that x_j is to be set to $x_j'' \pm a/2$ with equal probability.

Reference 1 gives a detailed description of efficient Monte Carlo algorithms to sample the distribution (91), the differential distribution (92) and the discrete distribution (93). These descriptions will not be repeated here.

VIII.2 The X^3 and Related Functions in the Case $\alpha_3^-=0$

The constant α_3^- is defined by Equation (52b). It is equal to the value $\alpha(x)$ appearing in Equation (6) and in Equation (3). The analysis up to now was completely general, assuming any non-negative value of α. Further analysis for $\alpha>0$ is not completed yet. We restrict, therefore, further discussion to the case $\alpha=0$, which applies to the case of known temperature boundary conditions as shown by Equation 2.

Let us first calculate the importance functions E and Q. The solution of Equations 56-57 for j=3, $a_3^- = -x_3'$, $a_3^+ = \infty, \alpha_3^{\pm} = 0$ is:

$$X^3(x,t) = \lim_{x'\to 0} \frac{1}{2\sqrt{\pi Dt}} \left[\exp(-x-x')^2/4Dt) - \exp(-(x+x')^2/4Dt\right] \tag{94}$$

Substituting that expression into Equation (60) one obtains:

$$E(x',t) = \frac{2}{\sqrt{\pi}} \int_{x'/2\sqrt{Dt}}^{\infty} e^{-u^2}\,du = \mathrm{erf}(x'/2\sqrt{Dt}) \tag{95}$$

Substituting Equation (94) into (66a) we obtain

$$E_s(x',t) = \mathrm{erf}(x'/2\sqrt{Dt}) \tag{95a}$$

The subscript ε can therefore be dropped in that case.

Substituting (94) into (62) and letting $x'\to 0$ one obtains

$$Q(0,t) = \frac{1}{\sqrt{\pi Dt}} \tag{96}$$

VIII.2.1 The Functions $p^3(t,t_0,x'')$, $r_v^3(x)$, $r_s^{3\pm}$

Let us consider the symmetric case $a_j^+ = -a_j^-$. The function $X^3(x,t)$ then satisfies the same set of equations as the function X^1 and X^2 discussed in Section VIII.1. In terms of the reduced variables (86) and (87) the solution is given by either Equation (89) or (90).

In terms of reduced variables, the importance function E (Equation (95) becomes:

$$E(\zeta,\tau) = \mathrm{erf}(\zeta/2\sqrt{\tau}) \qquad (97)$$

where $\zeta = 1/2 + \xi$ measures distances from the boundary. Let us substitute (97) and (88) into (64). For $\tau = \tau_0$ we obtain

$$F^{i}(\tau_0,\tau_0) = \frac{R(\tau_0)}{\mathrm{erf}(1/4\sqrt{\tau_0})} \qquad (98)$$

Making the same substitutions in Equation (66) we obtain:

$$p^{3}(\tau,\tau_0) = \frac{\mathrm{erf}(0/2\sqrt{\tau_0-\tau})\ \frac{-\partial}{\partial x}\ G(-\frac{1}{2},\tau) + \mathrm{erf}(1/2\sqrt{\tau_0-\tau})\ \frac{\partial}{\partial x}\ G(\frac{1}{2},\tau)}{\mathrm{erf}(1/4\sqrt{\tau_0})}$$

The first term vanishes as erf(0) = 0. Taking (93), (91a) and (67) into account, the above equation can be written as:

$$p^{3}(\tau,\tau_C) = \frac{\mathrm{erf}(1/2\sqrt{\tau_0-\tau})\ \frac{1}{2}\ \frac{-d}{d\tau}\ R(\tau)}{\mathrm{erf}(1/4\sqrt{\tau_0})} \qquad (99)$$

When $R(\tau)$ is defined by Equations 91b, 91c.

Algorithms to sample the time distribution (99) are discussed in Section IX.1.

Substituting (97) and (88) into Equation (69) we obtain:

$$r_v^{3}(\zeta) \propto \mathrm{erf}(\zeta/2\sqrt{\tau})\ G\ (\zeta-1/2,\tau) \qquad (100)$$

where $G(\xi,\tau)$ is given by Equation (89) or by Equation (90).

Algorithms to sample the spacial distribution (100) are discussed in Section IX.2.

Finally, Equation (72) becomes

$$r_s^{3-} = 0$$

The sampling of that discrete distribution is trivial.

VIII.2.2 The Functions $q^3(t,t_0)$ $S_v^3(x)$, $S_s^{3\pm}$

The Green's function $X^3(x_3,t)$ satisfies Equations (56)-(58) written for $j=3$, with $\alpha_3^{\pm} = 0$, $a_3^- = 0$ and $a_3^+ = a$.

Let us introduce the reduced variables

$$\zeta = x_3/a \tag{102}$$

$$\tau = Dt/a^2 \tag{103}$$

$$X^3(x_3,t)dx_3 = X(\zeta,\tau)d\zeta \tag{104}$$

In terms of these variables, Equations (56-58) become:

$$\frac{\partial^2}{\partial\zeta^2} X(\zeta,\tau) - \frac{\partial}{\partial\tau} X(\zeta,\tau) = 0 \tag{105}$$

$$X(\zeta,\tau) = 0 \quad \text{for } \zeta = 0,\ \zeta = 1 \tag{106}$$

$$X(\zeta,0) = \delta(\zeta) \tag{107}$$

The solution of (105)-(107) can be given in the form of an eigenfunction expansion:

$$X(\zeta-\zeta',\tau) = \lim_{\zeta'\to 0} 2 \sum_{m=1}^{\infty} \sin(m\pi\zeta')\sin(m\pi\zeta)\, e^{-m^2\pi^2\tau}$$

giving the expression

$$\lim_{\zeta'\to 0} \frac{\partial}{\partial\zeta'} X(\zeta-\zeta',\tau) = 2 \sum_{m=1}^{\infty} m\pi \sin(m\pi\zeta) e^{-m^2\pi^2\tau} \tag{108}$$

which converges rapidly for large τ.

The solution can also be given in the form of an image expansion

$$X(\zeta-\zeta',\tau) = \frac{1}{2\sqrt{\pi\tau}}\Bigg[\exp(-(\zeta-\zeta')^2/4\tau) - \exp(-\zeta+\zeta')^2/4\tau)$$

$$+ \sum_{n=1}^{\infty}\Bigg\{-\exp(-(\zeta+\zeta'-2n)^2/4\tau) + \exp(-(\zeta-\zeta'-2n)^2/4\tau)$$

$$+ \exp(-(\zeta-\zeta' + 2n)^2/4\tau) - \exp(-(\zeta+\zeta' + 2n)^2/4\tau)\Bigg\}\Bigg]$$

giving the expression

$$\lim_{\zeta'\to 0} \frac{\partial}{\partial\zeta'} X(\zeta-\zeta',\tau) = \frac{1}{2\tau\sqrt{\pi\tau}}\Bigg[\zeta \exp(-\zeta^2/4\tau) \tag{109}$$

$$+ \sum_{n=1}^{\infty}\Bigg\{-(2n-\zeta)\exp(-(2n-\zeta)^2/4\tau) + (2n+\zeta)\exp(-(2n+\zeta)^2/4\tau)\Bigg\}\Bigg]$$

which converges rapidly for small .

In terms of the reduced variables (102), (103), the expression of the importance functions are:

$$\left.\begin{aligned} E(\zeta,\tau) &= \operatorname{erf}(\zeta/2\sqrt{\tau}) \\ Q(0,\tau) &= \frac{1}{\sqrt{\pi\tau}} \end{aligned}\right\} \tag{110}$$

Substituting (110) and either (108) or (109) into Equation (74), we obtain the late and early time expansion of $H^3(t,t_0)$. The expressions are given in Appendix B. For $t = t_0$, an excellent approximation gives:

$$H^3(\tau_0,\tau_0) = 1 - 2e^{-1/4\tau_0} + 2e^{-1/\tau_0} \quad \text{for } \tau<\tau_e \tag{111a}$$

$$= 4\sqrt{\pi\tau_0}\, e^{-\pi^2\tau_0} \quad \text{for } \tau>\tau_e \tag{111b}$$

$$\tau_e = 0.225 \tag{111c}$$

corresponding to a relative error of less than one part in ten thousand.

Let us now rewrite Equation (76) in terms of the reduced variables (102), (103), taking expressions (110) into account.

$$q^3(\tau,\tau_0) = \sqrt{\pi\tau_0}\,\mathrm{erf}(1/2\sqrt{\tau_0-\tau})\ \frac{-\partial^2}{\partial\zeta^2}\,X(1,\tau) \tag{112}$$

In order to evaluate expression (112), let us start from the late time expression of $\frac{\partial}{\partial\zeta}$ $X(\zeta,t)$ (Equation 108) and calculate the derivative at $\zeta = 1$:

$$\frac{-\partial^2}{\partial\zeta^2}X(\zeta,\tau) = -\,2\sum_{n=1}^{\infty}(-1)^n\,n^2\pi^2\,e^{-n^2\pi^2\tau} \tag{112a}$$

or

$$\frac{-\partial^2}{\partial\zeta^2}X(\zeta,\tau) = \frac{-d}{d\tau}R(\tau) \tag{113}$$

where

$$R(\tau) = -2\sum_{n=1}^{\infty}(-1)^n\,e^{-n^2\pi^2\tau} \tag{114}$$

If, instead of the expansion (112a), we start from the early time expansion, we obtain:

$$\frac{-\partial^2}{\partial\zeta^2}X(\zeta,\tau) = \frac{-1}{2\tau\sqrt{\pi\tau}}\Bigg[(1-\frac{1}{2\tau})\exp(-1/4\tau)$$

$$+\sum_{n=1}^{\infty}\left\{(1-\frac{(2n-1)^2}{2\tau})\exp(-(2n-1)^2/4\tau)\right\}\Bigg]$$

$$+\ (1-\frac{(2n+1)^2}{2\tau})\exp(-(2n+1)^2/4\tau)$$

$$= \frac{-1}{\tau\sqrt{\pi\tau}}\sum_{n=1}^{\infty}(1-\frac{(2n-1)^2}{2\tau})\exp(-(2n-1)^2/4\tau)$$

an expression which can be brought into the form (113) with:

$$R(\tau) = 1 - \frac{2}{\sqrt{\pi\tau}}\sum_{n=1}^{\infty}\exp(-(2n-1)^2/4\tau) \tag{115}$$

Expressions (114) and (115) are defined within addition of an arbitrary (and irrelevant) constant. The constants have been chosen so that expressions (114) and (115) are different expansions of the same function of t, so that $R(t) = 0$ at $t = \infty$. It also happens that $R(0) = 1$. $R(t)$ (see Equation 113) can therefore be treated as a cumulative probability distribution function.

Substituting Equation (113) into (112) we obtain:

$$q^3(\tau,\tau_0) = \sqrt{\pi\tau_0}\ \mathrm{erf}(1/2\sqrt{\tau_0-\tau})\ \frac{-d}{d\tau} R(\tau) \tag{116}$$

where $R(t)$ is given by either Equation (114) or Equation (115). An excellent approximation is suggested:

$$R(\tau) = 1 - \frac{2}{\sqrt{\pi\tau}}\ e^{-1/4\tau} \qquad \text{for } \tau<\tau_e \tag{117a}$$

$$R(\tau) = 2\ e^{-\pi^2\tau} \qquad \text{for } \tau>\tau_e \tag{117b}$$

$$\tau_e = 0.225 \tag{117c}$$

The approximation provides at least four place accuracy for $0\leq\tau\leq\infty$.

Methods to sample $q^3(\tau,\tau_0)$ of Equation (116) are discussed in Section IX.1.

Writing Equation (79) in terms of the reduced variables (102), (103), we obtain:

$$S_v^3(\zeta) \propto \mathrm{erf}(\zeta/2\sqrt{\tau_0-\tau})\ \frac{\partial}{\partial\zeta} X(\zeta,\tau) \tag{118}$$

where $\frac{\partial}{\partial\zeta} X(\zeta,\tau)$ is given by Equation (108) or (109). We suggest that only the first two terms of Equation (108) be kept if $\tau>\tau_e$.

Methods to sample $q_3(\zeta)$ are discussed in Section IX.2.

Finally, Equation (82) reduces to:

$$S_s^{3-} = 0 \quad (119)$$

$$S_s^{3+} = 1 \quad (120)$$

Sampling of that discrete distribution is trivial.

IX. SAMPLING ALGORITHMS

IX.1 Sampling $p^3(\tau,\tau_0)$ and $q^3(\tau,\tau_0)$

Let us define the general function

$$p(\tau,\tau_0)d\tau = N(\tau_0)\cdot W\cdot \mathrm{erf}(1/2\sqrt{\tau_0-\tau})\cdot \frac{-d}{d\tau} R(\tau)d\tau \tag{121}$$

with a normalization

$$\int_0^{\tau_0} p(\tau,\tau_0)d\tau = 1 - N(\tau_0)R(\tau_0) \tag{122}$$

The function $p(\tau,\tau_0)$ can be made equal to $p^3(\tau,\tau_0)$ (Equation 99), by setting

$$N(\tau_0) = 1/\mathrm{erf}(1/4\sqrt{\tau_0}) \tag{123}$$

$$W = 1/2 \tag{124}$$

and defining $R(\tau)$ by Equations (91b-d).

Alternatively, the function $p(\tau,\tau_0)$ can be made equal to $q^3(\tau,\tau_0)$ (Equation 116) by setting

$$N(\tau_0) = H^3(\tau_0,\tau_0)/R(\tau_0) \tag{125}$$

$$W = \sqrt{\pi\tau_0}\; R(\tau_0)/H^3(\tau_0,\tau_0) \tag{126}$$

and defining $R(\tau)$ by Equations (117a-c).

The general sampling problem we discuss here is the following. With probability $F(\tau_0)$ set $\tau>\tau_0$; else sample τ from a renormalized $p(\tau,\tau_0)$.

Two different sampling algorithms are suggested, each having a different range of efficiency:

a. Small and Intermediate Values of τ_0

The following rejection technique is efficient:

Step 1 - Sample τ, $0<\tau<\infty$ from $\frac{-d}{d\tau} R(\tau)$.

If $\tau \geq \tau_0$, accept the sample.

If $\tau<\tau_0$ do the following:

Step 2 - With probability (1-w) reject the sample and repeat from Step 1. With remaining probability w do the following:

Step 3 - With probability $\mathrm{erf}(1/2\sqrt{\tau_0-\tau})$ accept the sample.

With remaining probability reject the sample and repeat from Step 1.

The probability of the algorithm producing an accepted time $\tau<\tau_0$ with $d\tau$ at the first step is equal to

$$w \, \mathrm{erf}(1/2\sqrt{\tau_0-\tau}) \, \frac{-d}{d\tau} R(\tau) d\tau$$

which is indeed proportional to the distribution (122).

The probability of rejecting the first sample is equal to

$$\int_0^{\tau_0} \left[1-w\cdot\mathrm{erf}(1/2\sqrt{\tau_0-\tau})\right] \frac{-d}{d\tau} R(\tau)d\tau$$

$$= 1 - R(\tau_0) - \frac{1}{N(\tau_0)} \left[1 - N(\tau_0)R(\tau_0)\right]$$

$$= 1 - \frac{1}{N(\tau_0)}$$

The efficiency of the algorithm is therefore equal to $1/N(\tau_0)$. The probability of sampling $\tau<\tau_0$ within $d\tau$ is not only proportional, but equal to the distribution (122).

The efficiency $1/N(\tau_0)$ is 100% for $\tau_0 \to 0$. In both cases of Equations (125) and (126), it is assymptotically $w/\sqrt{\pi\tau_0}$ for large τ_0. It becomes unacceptable for large values of τ_0.

Step No. 3 involves a game of chance with probability $\mathrm{erf}(1/2\sqrt{\tau_0-\tau})$, with both τ_0 and τ given. The following algorithm can be used:

Sample a Gaussian variable X $(p(x) = \frac{2}{\sqrt{\pi}} e^{-x^2} dx,\ 0<x<\infty)$. Set $\tau_1 = \tau_0 - 1/4x^2$. The probability that $\tau > \tau_1$ is $\mathrm{erf}(1/2\sqrt{\tau_0-\tau})$.

The details of sampling in the case of Equation (125) and (126) will be given in Section IX.1.1 and .2, respectively.

b. <u>Large and Intermediate Values of τ_0</u>

The algorithm just described involved a rejection technique based on the inequality $\mathrm{erf}(x) \leq 1$, which becomes assymptotically an equality as $x\to\infty$. We now propose to take advantage of another inequality, $\mathrm{erf}(x) \geq \frac{2}{\sqrt{\pi}} x$, which becomes assymptotically an equality as $x\to 0$. Having that in mind, we rewrite Equation (121) in the form:

$$p(\tau,\tau_0) = N_1 \cdot f_1(\tau) \cdot f_2(\tau) \tag{127}$$

where

$$f_1(\tau) = \sqrt{\pi(\tau_0-\tau)}\ \ \mathrm{erf}(1/2\sqrt{\tau_0-\tau}) \tag{128}$$

$$f_2(\tau) = f_3(\tau)/M \tag{129}$$

$$f_3(\tau) = \frac{w}{\sqrt{\pi(\tau_0-\tau)}} \frac{-d}{d\tau} R(\tau) \qquad \tau<\tau_0 \tag{130a}$$

$$= -\frac{d}{d\tau} R(\tau) \qquad \tau \geq \tau_0 \tag{130b}$$

$$M = \int_0^\infty f_3(\tau)d\tau \tag{131}$$

$$N = N(\tau_0)/M. \tag{132}$$

Similarly, Equation (128) can be rewritten as:

$$\int_0^{\tau_0} p(\tau,\tau_0)d\tau \quad 1 - N_1 \int_{\tau_0}^{\infty} f_2(\tau)d\tau \quad . \tag{133}$$

To sample Equation (127), we propose the following rejection technique:

Step 1 - Sample t, $0<t<\infty$, from $f_2(\tau)$. If $t \geq t_0$, accept the sample. If $t<t_0$, do the following:

Step 2 - With probability $f_1(\tau)$ accept the sample. Else reject the sample and repeat from Step 1.

The efficiency of the technique is 100% for $\tau_0 \to \infty$, but deteriorates for small values of τ_0.

Step No. 2 involves a game of chance with probability $f_1(\tau)$ defined by Equation (128). In order to construct an appropriate algorithm, let

$$x = 1/4(\tau_0 - \tau)$$

In terms of x, the probability (128) becomes

$$f_1 = \frac{1}{2}\sqrt{\frac{\pi}{x}}\, \mathrm{erf}(\sqrt{x}) \tag{134}$$

Equation (134) can be expanded in Taylor series:

$$f_1 = 1 - \frac{x}{3} + \frac{x^2}{2!5} - \frac{x^3}{3!7} = --- = \frac{(-x)^n}{n!(2n+1)} + --- \tag{135}$$

for $x<3$ the absolute value of each term of the expansion (135) is smaller than that of the preceding term. This property permits the use of a particularly simple algorithm:

Set n=1, set u = a random number

Step 1 - Set $u = u - X^n/(n!(2n+1))$. Accept the sample if $u \geq 0$. If $u<0$, perform the next step.

Step 2 - Set $u = u + X^{n+1}/((n+1)!(2n+2))$. Reject the sample if $u \leq 0$. If $u>0$, set n=n+2 and perform Step 1.

If $x \geq 3$ (which is a rave event), we take advantage of the semi convergent expansion

$$f_1 = \frac{\sqrt{\pi}}{2\sqrt{x}} - \frac{e^{-x}}{2x}\left(1 - \frac{1}{2x} + \frac{1.3}{(2x)^2} + \text{---} + \frac{1.3. \text{ -- } (2n-1)}{(-2x)^n}\right) \qquad (136)$$

The expansion has the property that, if truncated, the remainder is less than the absolute value of the first term neglected, and of the same sign. This property permits the following algorithms:

Set u_0 = a random number

Step 1 - Set $u = u_0$

Step 2 - Set $u = \frac{1}{2}\sqrt{\frac{\pi}{x}} - u$. Reject the sample if $u \leq 0$. If $u>0$, perform the next step.

Step 3 - Set $u = u \cdot x \cdot e^x - 1$. Accept the sample if $u \geq 0$. If $u<0$, set $u = u.2/\sqrt{\pi}$, set $n = 1$ and perform the next step.

Step 4 - Set $u = u + (1.3. \text{ --- } (2n-1))/(2x)^n$. Reject the sample if $u \leq 0$. If $n>0$, perform the next step.

Step 5 - Set $u = u - (1.3. \text{ --- } (2n+1))/(2x)^{n+1}$. Accept the sample if $u \geq 0$. If $u<0$, set $n = n+2$ and perform Step 6.

Step 6 - If $n<X + 1/2$ repeat Step 4. If not, perform Step 7.

Step 7 - Calculate $\mathrm{erf}(\sqrt{x})$ by other means. Accept the sample if $u_0 < \frac{1}{2}\sqrt{\frac{\pi}{x}}\,\mathrm{erf}(\sqrt{x})$. Reject the sample otherwise.

The test on n performed in Step 6 corresponds to truncation of expansion (136) corresponding to a minimum remainder. Given $x \geq 3$, the probability of executing Step 7 (and therefore of having to calculate $\mathrm{erf}(\sqrt{x})$) is less than $\exp(-3) \cdot 3 \cdot 5/6^4 < 0.0006$.

The details of sampling in the case of Equations (123,124) and (125,126) will be given in Section IX.1.1 and .2, respectively.

IX.1.1 Details for Sampling $p^3(\tau, \tau_0)$

a. Small and Intermediate Values of τ_0

The general method is described in Section IX.1.a. Detailed algorithms for sampling $\frac{-d}{dt}$ R(t) are given in Section III.4 of Reference 1.

b. Large and Intermediate Values of τ_0

The general method is described in Section IX.1.b. We now will work out a detailed sampling technique in the particular case of $R(\tau)$ as given by Equation (91b-c). As defined in these equations, R(t) has different functional forms for $\tau<\tau_e$ and $\tau>\tau_e$ (τ_e is defined to be equal to 0.05 by Equation 91d). We will assume that $\tau_e<\tau_0$, and derive the expression of $f_3(\tau)$ (Equation 130) in the three cases $0<\tau<\tau_e$, $\tau_e<\tau<\tau_0$, $\tau_0<\tau$.

- α. The Case $0<\tau<\tau_e$

Substituting Equation (124) and (91b) into (130a) we obtain

$$f_3(\tau)d\tau = \frac{1}{2\sqrt{\pi(\tau_0-\tau)}} \frac{-d}{d\tau} \left[1 - \frac{4}{\sqrt{\pi}} \int_{1/4\sqrt{\tau}}^{\infty} e^{-u^2} du \right] d\tau \tag{137}$$

Let us perform the change of variables

$$v = 1/4\sqrt{t} - v_e \tag{138}$$

where $v_e = 1/4\sqrt{\tau_e}$

Equation (137) becomes

$$f_3(v)dv = \frac{2}{\pi\sqrt{\tau_0-\tau}} e^{-(v+v_e)^2} dv \tag{139}$$

which we rewrite in the form

$$f_3(v)dv = \alpha_e\, g_e\, h_e(v)dv \qquad (140a)$$

with

$$\alpha_e = \frac{4}{\pi}\sqrt{\frac{\tau_e}{\tau_0-\tau_e}}\; e^{-1/16\tau_e} \qquad (140b)$$

$$g_e = \sqrt{\frac{\tau_0-\tau_e}{\tau_0-\tau}}\; e^{-v^2} \qquad (140c)$$

$$h_e(v)dv = e^{-2v_e v}\; 2v_e dv \qquad (140d)$$

$$v_e = 1/4\sqrt{\tau_e}\ ;\ \tau = 1/(4v - 4v_e)^2 \qquad (140e)$$

$h_e(v)$ is properly normalized in its range *$0<v<\infty$ corresponding to $\tau_e>\tau>_0$, and* $0\le g_e\le 1$.

- β. <u>The Case $\tau_e<\tau<\tau_0$</u>

Substituting Equation (126) and (91c) into (130a) we obtain

$$f_3(t) = \frac{1}{2\sqrt{\pi(\tau_0-\tau)}}\ \frac{4}{\pi}\ \frac{-d}{d\tau}\ (e^{-\pi^2\tau} - \frac{1}{3}\,e^{-q\pi^2\tau}) \qquad (141)$$

$$= 2\sqrt{\frac{\pi}{\tau_0-\tau}}\; e^{-\pi^2\tau}\quad (1-3e^{-8\pi^2\tau})$$

Let us perform the change of variables $u = \pi\sqrt{t_0-t}$.

Equation (141) becomes

$$p(u)du = \frac{4}{\sqrt{\pi}}\,(1 - 3e^{-8\pi^2 t})\; e^{-\pi^2 t_0 + u^2}\; du \qquad (142)$$

Performing the change of variable $u = u_e - v$, where $u_e = \pi\sqrt{\tau_0 - \tau_e}$, Equation (142) becomes

$$p(v)dv = \frac{4}{\sqrt{\pi}} (1 - 3e^{-8\pi^2 t})\, e^{-\pi^2 t_0 + (u_e - v)^2} dv$$

which we rewrite in the form

$$p(v)dv = \alpha_\ell\, g_\ell\, h_\ell(v)dv \tag{143a}$$

where

$$\alpha_\ell = 4(e^{-\pi^2 \tau_e} - e^{-\pi^2 \tau_0})/(\sqrt{\pi}\, u_e) \tag{143b}$$

$$g_\ell = (1 - 3e^{-8\pi^2 \tau})\, e^{-v(u_e - v)} \tag{143c}$$

$$h_\ell(v)dv = \frac{e^{-u_e v}\, u_e dv}{1 - e^{-u_e^2}} \tag{143d}$$

$$u_e = \pi\sqrt{\tau_0 - \tau_e} \quad ; \quad t = t_0 - (u_e - v)^2/\pi^2 \tag{143e}$$

$h_\ell(v)$ is properly normalized in its range $0 < v < u_e$ corresponding to $\tau_0 > \tau > \tau_e$, and $0 \leq g_e \leq 1$.

- γ. <u>The Case $\tau > \tau_0 > \tau_e$</u>

Substituting (91c) into (130b) we obtain

$$f_3(t) = \frac{4}{\pi} \frac{-d}{d\tau} (e^{-\pi^2 \tau} - \frac{1}{3} e^{-q\pi^2 \tau}) \tag{144}$$

Making the change of variables $v = t - t_0$, we obtain an equation which we write as

$$f_3(v)dv = \alpha_0\, g_0\, h_0(v)dv \tag{145a}$$

where

$$\alpha_0 = \frac{4}{\pi}\, e^{-\pi^2 t_0} \tag{145b}$$

$$g_0 = 1\text{-}3\, e^{-\pi^2 t} \tag{145c}$$

$$h_0(v)dv = e^{-\pi^2 v}\, \pi^2 dv \tag{145d}$$

$h_0(v)$ is properly normalized in its range, and $0 \le g_0 \le 1$.

Let us now compute the results of subsection α, β, and γ:

$f_3(t)$ is given by an expression

$$A\left[\beta_e g_e h_e(v) + \beta_\ell g_\ell h_\ell(v) + \beta_0 g_0 h_0(v)\right] dv \tag{146}$$

where

$$A = \alpha_e + \alpha_\ell + \alpha_0 \quad \text{and} \quad \beta_r = \alpha_r/A \text{ for } r=e, \ell, 0.$$

To sample expression (146), one samples range "r" with probability β_r ($r=e, \ell, 0$). Given the range r, one samples $h_r(v)dv$, performs the proper change of variable to obtain a time τ, and calculates g_r. With probability g_r the sample τ is accepted as a valid sample of $f_2(\tau)$ defined by Equation (129). In case of rejection, a new attempt to sample is made, starting from sampling the range "r".

It happens that all the distributions $h_r(v)dv$ are exponential which can be sampled by standard methods.

IX.1.2 Details for Sampling $q^3(\tau,\tau_0)$

a. Small and Intermediate Values of τ_0

The general method is described in Section IX.1.a. We will now work out detailed schemes to sample $\frac{-d}{d\tau} R(\tau)$ with $R(\tau)$ given by Equations (117). Two cases are to be considered depending on $\tau<\tau_m$ or $\tau>\tau_m$, where $\tau_m = \min(\tau_e,\tau_0)$.

- α. The Case $0<\tau<\tau_m$

$$p(\tau)d\tau = -\frac{d}{d\tau} R(\tau)d\tau = -\frac{d}{d\tau}\left[1-\frac{2}{\sqrt{\pi\tau}}e^{-1/4\tau}\right]d\tau \tag{147}$$

Let $u = 1/2\sqrt{\tau}$; $u_e = 1/2\sqrt{\tau_m}$

$$p(u)du = -\frac{4}{\sqrt{\pi}}\frac{d}{du}(u\,e^{-u^2})du = \frac{4}{\sqrt{\pi}}(2u^2-1)e^{-u^2}\,du$$

Let $u = u_e + w$

$$p(w)dw = \frac{4}{\sqrt{\pi}}(2u_e^2 - 1 + 4u_e\,w + 2w^2)\,e^{-u_e^2-2u_e w-w^2}\,dw$$

Let $v = 2u_e w$

$$p(v)dv = \alpha_e\,g_e\,h_e(v)dv \tag{148a}$$

where

$$\alpha_e = \frac{2}{\sqrt{\pi\tau_m}}e^{-\frac{1}{4\tau_m}}(1 + 2\tau_m + 8\tau_m^2) \tag{148b}$$

$$g_e = e^{-\tau_m v^2} \tag{148c}$$

$$h_e(v) = \sum_{v=1}^{3} p_i q_i(v)dv \tag{148d}$$

$$\left.\begin{array}{ll} q_1(v) = e^{-v} & ;\quad p_1 = (1-2\tau_m)/(1+2\tau_m+8\tau_m^2) \\ q_2(v) = ve^{-v} & ;\quad p_2 = 4\tau_m/(1+2\tau_m + 8\tau_m^2) \\ q_3(v) = \frac{v^2}{2}e^{-v} & ;\quad p_3 = 8\tau_m^2/(1+2\tau_m + 8\tau_m^2) \end{array}\right\} \tag{148e}$$

$$\tau = \tau_m/(1 + 2\tau_m v)^2$$

To sample $h_e(v)$ defined by Equation (148d), we set $v = -\log(y)$ where y is the product of 1, 2, or 3 random numbers with probability p_1, p_2, p_3, respectively.

- β. The case $\tau_m < \tau$

$$p(\tau)d\tau = -\frac{d}{d\tau} R(\tau)d\tau = -\frac{d}{d\tau} 2e^{-\pi^2\tau}d \quad (149)$$

Let $v = \tau - \tau_m$

$$p(v)dv = \alpha_\ell g_\ell h_\ell(v)dv \quad (150a)$$

where

$$\alpha_\ell = 2e^{-\pi^2\tau_m} \quad (150b)$$

$$g_\ell = 1 \quad (150c)$$

$$h_\ell(v)dv = e^{-\pi^2 v}\pi^2 dv \quad (150d)$$

$$\tau = \tau_m + v \quad (150e)$$

Recapitulating the results, the time distribution is written in the form

$$A\left[\beta_e\, g_e\, h_e(v) + \beta_\ell\, g_\ell\, h_\ell(v)\right]$$

where

$$A = \alpha_e + \alpha_\ell \;,\quad \beta_e = \alpha_e/A \;,\quad \beta_\ell = \alpha_\ell/A$$

To sample, one first samples a range (e or ℓ) with probability β_e and β_ℓ, respectively. Once the range r is given, one samples v from the appropriate distribution $h_r(v)$. Given v, one accepts the sample with probability g_r. In case of rejection, the complete sampling is repeated.

In practice, it was found efficient to slightly modify the general technique described in Section IX.1.a. α_e is multiplied by w (defined by Equation 126b). The game of chance based on w described in Step 2 of that section can then be bypassed.

- ℓ. Large and Intermediate Values of τ_0

The general method is described in Section IX.1.b. In the case under consideration $R(\tau)$ is defined by Equations (117a-c); it has different functional forms for $\tau<\tau_e$ and $\tau>\tau_e$. We will assume $\tau_e<\tau_0$. Three cases are to be considered.

- α. The Case $0<\tau<\tau_e$

Substituting (126b) and (117a) into (130a) we obtain:

$$f_3(\tau)d\tau = \frac{1}{2}\frac{1}{\sqrt{\pi(\tau_0-\tau)}}\frac{-d}{d\tau}\left[1-\frac{2}{\sqrt{\pi\tau}}e^{-1/4\tau}\right]d\tau \tag{151}$$

Performing the same operations as in subsection b, we can rewrite (Equation 151) in the form

$$f_3(\tau)d\tau = \alpha_e\, g_e\, h_e(v)dv \tag{152a}$$

where

$$\alpha_e = \frac{1}{\pi\sqrt{\tau_e(\tau_0-\tau_e)}}\left[1+2\tau_e+8\tau_e^{\,2}\right]e^{-1/4\tau_e} \tag{152b}$$

$$g_e = \sqrt{\frac{\tau_0-\tau_e}{\tau_0-\tau}}\quad e^{-\tau_e v^2} \tag{152c}$$

$$h_e(v)dv = q(r)dv \tag{152d}$$

$$v = \frac{1}{2\sqrt{\tau_e}}\left[\frac{1}{\sqrt{\tau}}-\frac{1}{\sqrt{\tau_e}}\right] \tag{152e}$$

where q(v) is given by Equations (149-150).

- β. <u>The Case $\tau_e<\tau<\tau_0$</u>

Substituting (126b) and (117b) into (130a), we obtain:

$$f_3(\tau)d\tau = \frac{1}{2} \frac{1}{\sqrt{\pi(\tau_0-\tau)}} \frac{-d}{d\tau} \left[2e^{-\pi^2\tau}\right] d\tau \qquad (153)$$

Equation (153) is quite similar to Equation (141) of Section IX.1.1.b.β. Performing the same operations as in that section, Equation (153) is rewritten in the form:

$$f_3(t)dt = \alpha_\ell \; g_\ell \; h_\ell(v)dv \qquad (154a)$$

where

$$\alpha_\ell = \frac{2\sqrt{\pi}}{u_e} \left[e^{-\pi^2\tau_e} - e^{-\pi^2\tau_0}\right] \qquad (154b)$$

$$g_\ell = e^{-v(u_e-v)} \qquad (154c)$$

$$h_\ell(v)dv = \frac{e^{-u_e v} \; u_e dv}{1-e^{-u_e^2}} \qquad (154d)$$

$$u_e = \pi\sqrt{\tau_0-\tau_e} \quad ; \quad t = t_0 - (u_e-v)^2/\pi^2 \qquad (154e)$$

- γ. <u>The Case $\tau>\tau_0$</u>

Substituting (117b) into (130b) we obtain:

$$f_3(\tau)d\tau = \frac{-d}{d\tau} \left[2e^{-\pi^2\tau}\right] \qquad (155)$$

which we write in the form

$$p_3(\tau) = \alpha_0 \; g_0 \; h_0(v)dv \qquad (156a)$$

where

$$\alpha_0 = 2e^{-\pi^2\tau_0} \tag{156b}$$

$$g_0 = 1 \tag{156c}$$

$$h_0(v)dv = e^{-\pi^2 v}\,\pi^2 dv \tag{156d}$$

$$v = \tau-\tau_0 \tag{156e}$$

Recapitulating the results of subsections α, β, and γ, the distribution $f_3(t)$ is given by expression (146). The sampling scheme given at the end of Section IX.1.1 applies.

IX.2 Sampling $r_v^3(\zeta)$ and $S_v^3(\zeta)$

$r_v^3(\zeta)$ is defined by Equation (100). $S_v^3(\zeta)$ is defined by Equation (118). Let us define the general distribution function

$$p(\zeta)d\zeta \propto \mathrm{erf}(\zeta/2\sqrt{\tau_0-\tau})\ r(\zeta)d\zeta \tag{157}$$

$p(\zeta)$ becomes equal to $r_3^3(\zeta)$ if $r(\zeta)$ becomes equal to $G(\zeta-1/2,\tau)$ as defined by Equation (89) or (90). $p(\zeta)$ becomes equal to $S_v^3(\zeta)$ if $r(\zeta)$ becomes equal to $\frac{\partial X}{\partial \zeta}(\zeta,\tau)$ as defined by Equation (108) or (109).

Two different sampling algorithms are suggested, each having a different efficiency in different ranges.

- a. Small and Intermediate Values of $\tau_0-\tau$

Step 1. Sample ζ, $0<\zeta<1$, from $r(\zeta)$

Step 2. With probability $\mathrm{erf}(\zeta/2\sqrt{\tau_0-\tau})/\mathrm{erf}(1/2\sqrt{\tau_0-\tau})$ accept the sample. With remaining probability reject the sample and start from Step 1.

The efficiency of the rejection technique is 100% for $\tau=\tau_0$, but becomes poor for large values of $\tau_0-\tau$.

The game of chance in Step #2 can be implemented as follows. Sample X, $0<X<1/2\sqrt{\tau_0-\tau}$ from a truncated Gaussian $(e^{-x^2}dx/\mathrm{erf}(1/2\sqrt{\tau_0-\tau})$. Accept the sample ζ if $\zeta> 2\sqrt{\tau_0-\tau}\ x$.

- b. <u>Large and Intermediate Values of $\tau_0-\tau$</u>

In this range of $\tau_0-\tau$, we rewrite Equation (157) in the form

$$p(\zeta) \propto f_1(\zeta)\ f_2(\zeta)d\zeta \tag{158}$$

where

$$f_1(\zeta) = \mathrm{erf}(\zeta/2\sqrt{\tau_0-\tau})\ \sqrt{\pi(\tau_0-\tau)}/\zeta \tag{159}$$

and

$$f_2(\zeta) \propto \zeta r(\zeta)d\zeta \tag{160}$$

As in Section IX.1.b, we propose to sample ζ from $f_2(\zeta)$ and accept the sample with probability $f_1(\zeta)$. An efficient algorithm to implement the latter is described at the end of Section IX.1.b.

The efficiency of the rejection technique is 100% as $\tau_0-\tau\to\infty$. It becomes poor for small values of $\tau_0-\tau$.

IX.2.1 <u>Details for Sampling $r_v^3(\zeta)$</u>

- a. <u>Small and Intermediate Values of $\tau_0-\tau$</u>

The general technique is described in Section IX.2.a. The technique involves sampling $r(\zeta)$ which is equal to $G(\zeta-1/2,t)$. Algorithms to perform that sampling are described in Section III.4 of reference 1.

- b. <u>Large and Intermediate Values of $\tau_0-\tau$</u>

The general technique is described in Section IX.2.b. It involves sampling $f_2(\zeta) \propto \zeta G(\zeta-1/2,t)$.

As $G(\xi,t)$ is an even function of ξ, the sampling of $f_2(\zeta)$ can be performed as follows:

1. Sample ξ, $-1/2<\xi<1/2$, from $G(\xi,\tau)$
2. Set $\zeta = 1/2 + \xi$
3. Accept the sample ζ with probability ζ. Else, set $\zeta = 1/2 - \xi$.

Methods to sample G are given in Section III.4 of reference 1.

IX.2.2 Details for Sampling $S_v^3(\zeta)$

- a. Small and Intermediate Values of $\tau_0-\tau$

The general technique is described in Section IX.2.a. It involves sampling $r(\zeta) = \frac{\partial X}{\partial \zeta}(\zeta,\tau)$ as defined by Equation (108) or (109).

- α. Case of Early Times ($\tau<\tau_e$, $\tau_e=0.225$)

At early times we propose to use Equation (109). In terms of the variables

$$u = \zeta/2\sqrt{\tau} \quad ; \quad u_0 = 1/2\sqrt{\tau} \tag{161}$$

Equation (109) becomes:

$$r(\zeta)d\zeta = p(u)du = 2ue^{-u^2}\,du + \sum_{n=1}^{\infty} -2(2n\,u_0-u)e^{-(2n\,u_0-u)^2} + 2(2n\,u_0 + u)e^{-(2n\,u_0+u)^2}\,du \tag{162}$$

or:

$$p(u)du = 2e^{-u^2}\left\{u - \sum_{n=1}^{\infty}(u_n^- - u_n^+)\right\}du \tag{163}$$

where

$$u_n^{\pm} = (2n\,u_0 \pm u)\,e^{-4n\,u_0(n\,u_0 \pm u)} \tag{164}$$

If $u_0>1/2$ (i.e., $\tau<1$, which is true in our case of small τ), $u_n^- - u_n^+ \geq 0$ for all n. This implies

$$p(u)du \leq 2ue^{-u^2}\,du,$$

which suggests the following rejection technique:

1. Sample u, $0<u<u_0$, from $2ue^{-u^2}du$. This can be done by sampling a random number ξ and setting $u = [\mathrm{Mod}(-\log(\xi), u_0^2)]^{1/2}$.

2. Let v = u

3. Sample a random number ξ and set $w = \xi \cdot u$

4. Set n = 1

5. Calculate u_n^-. If $u_n^- > v$ jump to Step #8. Else:

6. If $u_n^- \leq w$ the sample u is accepted (the sampling is completed). Else:

7. Calculate u_n^+. If $u_n^+ < w$ the sample is rejected. Repeat from Step #1. Else jump to Step #9.

8. Calculate u_n^+ and set $v = v - u_n^- + u_n^+$. If $v<w$ the sample is rejected. Repeat from Step #1. Else:

9. Set n = n+1 and repeat from Step #5.

Step #1 involves the sampling of $2ue^{-u^2}du$. It remains to be shown that Steps #2-9 correspond to an acceptance probability of $1 - \frac{1}{u} \sum_{n=1}^{\infty} (u_n^- - u_n^+)$.

Let us consider the rejection probability for each value of n. If Steps 6 and 7 are executed, rejection occurs if a random variable w, uniformly distributed between 0 and u satisfies $u_n^+ < w < u_n^-$ (<u). This has probability $(u_n^- - u_n^+)/u$. If Step No. 8 is executed, rejection occurs if the random variable w satisfies $v-u_n^- + u_n^+ < w < v(<u)$. This has also probability $(u_n^- - u_n^+)/u$.

Summed over all n, the rejection probability is indeed $\frac{1}{u} \sum_{n=1}^{\infty} (u_n^- - u_n^+)$. As the acceptance probability is equal to unity minus the rejection probability, the proof can be considered as completed.

An instructive though lengthy proof consists in examining the acceptance probability for each value of n. The acceptance probability for n = 1 is either zero (if Step #8 is executed), or $(u-u_n^-)/u$ if Step #6 is executed (as $u_n^- < w < u$ has that probability). If it is zero for n=1, it remains as zero for the succeeding n's, up to and including the smallest value of n, $n=n_0$, for which

$$v_0 = u = \sum_{n=1}^{n_0} (u_n^- - u_n^+) > u_{n_0+1}^-$$

For $n = n_0 + 1$, the acceptance probability is

$$\frac{1}{u}(v_0 - u_{n_0+1}^-)$$

(as $u_{n_0+1}^- < w < v_0$ has that probability).

For all $n>n_0 + 1$, the acceptance probability is

$$\frac{1}{u}(u_{n-1}^+ - u_n^-)$$

(as $u_n^- < w < u_{n-1}^+$ has that probability).

Summed over all n's, the acceptance probability is

$$\frac{1}{u}(v_0 - u_{n_0+1}^-) + \frac{1}{u}\sum_{n=n_0+2}^{\infty}(u_{n-1}^+ - u_n^-)$$

$$= \frac{1}{u}\left[u = \sum_{n=1}^{\infty}(u_n^- - u_n^+)\right. \qquad \text{QED.}$$

- β. Case of Late Times ($\tau > \tau_e$)

At late times, $r(\zeta)$ is given by Equation (108). Keeping only the first two terms, we obtain:

$$r(\zeta)d\zeta \propto 2\pi\left[e^{-\pi^2\tau}\sin\pi\zeta + 4e^{-4\pi^2\tau}\sin 2\pi\zeta\right]d\zeta$$

$$\propto \left[\sin(\pi\zeta) + \varepsilon\cos(\pi\zeta)\sin(\rho\zeta)\right]\pi d\zeta \qquad (165)$$

where $\varepsilon = 8e^{-3\pi^2\tau}$

Let $\cos(\pi\zeta) = 2x-1$. Equation (165) becomes

$$r(x)dx = (1-\varepsilon)dx + \varepsilon\ 2xdx \tag{166}$$

To sample (166) one can do the following.

With probability $(1-\varepsilon)$, x is set to a random number. With remaining probability, x is set to the largest of two random numbers. Once x is sampled:

$$\zeta = \cos^{-1}(2x-1)/\pi \tag{167}$$

- b. Large and Intermediate Values of $\tau_0-\tau$

The general technique is described in Section IX.2.b. $p_2(\zeta)$ is proportional to $\zeta r(\zeta)$, where $r(\zeta)$ has been discussed above.

- α. Case of Early Times ($\tau<\tau_e$)

The early time behavior of $r(\zeta)$ has been discussed in Section IX.2.2.a.α. Performing the change of variable $u = \zeta/2\sqrt{\tau}$ we obtain:

$$r(\zeta)d\zeta \propto u\ p(u)du$$

where p(u) is given by Equation (163).

The technique described to sample p(u) can be easily modified to sample u p(u)du. Only the first step of the rejection techniques needs to be modified. Instead of sampling $\propto ue^{-u^2}du$, one samples $\propto u^2e^{-u^2}du$, which can be achieved by setting

$$u = \sqrt{-\log(\xi_1)\ \sin^2(\pi\xi_2)-\log(\xi_2)}$$

and accepting the sample of $u\leq u_0$.

The remainder of the rejection technique applies without modification.

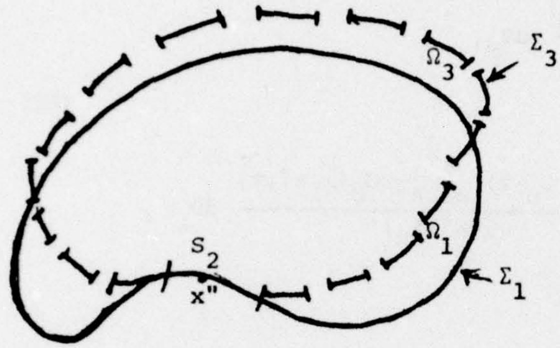
- β. Case of Late Times ($\tau>\tau_e$)

At late times, we propose a simple rejection technique:

1. Sample $r(\zeta)$ as discussed in Section IX.2.2.a.β, $0<\zeta<1$.
2. Accept with probability ζ. Else reject and repeat Step 1.

APPENDIX A

A Crucial Inequality

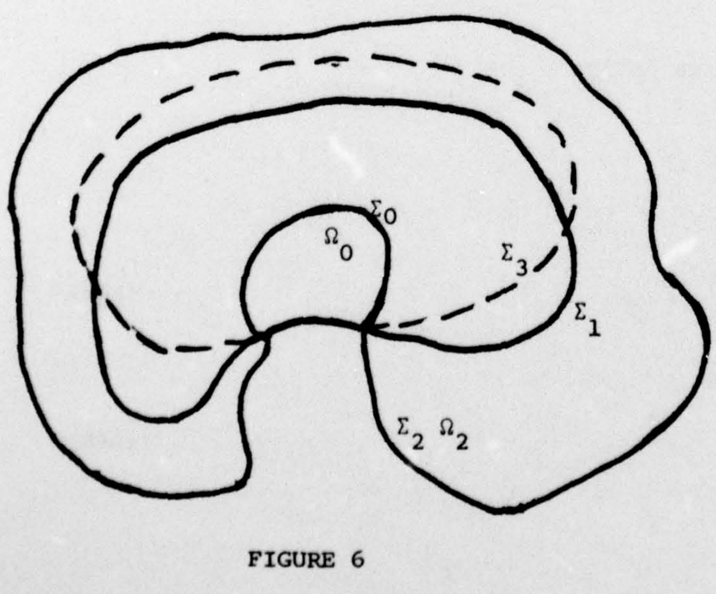


Let Ω_1 be a volume surrounded by surface Σ_1. Let x" be a point on Σ_1. (See Figure 6). Let Ω_3 be a volume surrounded by surface Σ_3, such that Σ_1 and Σ_3 are tangent at x", with the same outer normal. Let S_2 be the surface common to Σ_1 and Σ_3 (S_2 can degenerate to the single point x"), And let $S_{1i} = \Sigma_1 \quad S_2$ for i=1 and i=3.

Let G_1 and G_3 be Green's functions satisfying Equations (4,5,6) for i=1 and 3, respectively.

We are going to prove the following inequality:

$$\frac{\displaystyle\int_{\Omega_1} -\frac{\partial}{\partial n''} G_1(x'',x,t)\,dV_x}{\displaystyle\int_{\Omega_3} -\frac{\partial}{\partial n''} G_3(x'',x,t)\,dV_x} < \infty \qquad \text{for } 0 \leq t \leq t_0 < \infty \tag{A1}$$



Let us introduce a surface $\Sigma_0 = S_{1,0} + S_2$ surrounding a volume Ω_0. $S_{1,0}$ is completely internal to both Σ_1 and Σ_3. Let us also introduce a surface $\Sigma_2 = S_{1,2} + S_2$ surrounding a volume Ω_2. $S_{1,2}$ is completely external to both Σ_1 and Σ_2.

FIGURE 6

Equation (42) of Section IV has been derived without assuming (A1). Let us consider that equation for i=1 and 3, and integrate both sides over the volume Ω_i. We obtain:

$$\frac{Q_i(x",t_0)}{Q(x",t_0)} = \int_{\Omega_0} \frac{-\frac{\partial}{\partial n"} G_0(x',x",t_0)}{Q(x",t_0)} dV_{x'}$$

$$+\int_0^{t_0} dt \int_{S_{1,0}} \frac{E_i(x,t_0-t)}{E_{x"}(x,t_0-t)} \frac{E_{x"}(x,t_0-t)\frac{\partial^2}{\partial n \partial n"} G_0(x,x",t)}{Q(x",t_0)} dS_x \qquad \text{(A2)}$$

where

$$E_i(x,t) = \int_{\Omega_1} G_i(x,x',t)dV_{x'} \qquad \text{(A3)}$$

$$Q_i(x",t_0) = \int_{\Omega_i} -\frac{\partial}{\partial n"} G_i(x",x',t_0)dV_{x'} \qquad \text{(A4)}$$

As the solutions of the set of equations (4-6) are positive, we have

$G_i(x,x',t_0) \geq 0$ for $x,x' \epsilon \Omega_i$.

This implies

$$E_i(x,t) \geq 0. \qquad \text{(A3a)}$$

From the boundary condition (6) we derive

$$\frac{-\partial}{\partial n} G_i(x,x',t) = \frac{1}{\alpha(x)} G_i(x,x',t_0) \geq 0$$

which implies

$$Q_i(x,t) \geq 0 \qquad \text{(A4a)}$$

Furthermore, we can show that for $t<\infty$

$$Q_i(x,t) > 0 \quad \text{for } t<\infty. \qquad \text{(A4b)}$$

According to Equation (10) and (A3) we also have

$$Q(x'',t_0) = Q_2(x'',t_0) \tag{A5}$$

and, according to Equation (13) and (A4):

$$E_{x''}(x,t) = E_2(x,t) \tag{A6}$$

From (A2) we can derive the upper bound

$$\frac{Q_1(x'',t_0)}{Q(x'',t_0)} \leq A + B\cdot U(E_1/E_2) \tag{A7}$$

and the lower bound

$$\frac{Q_3(x'',t_0)}{Q(x'',t_0)} \geq A + B\cdot L(E_3/E_2) \tag{A8}$$

where

$$A = \int_{\Omega_0} \frac{-\frac{\partial}{\partial n''} G_0(x',x'',t_0)}{Q(x'',t_0)} dV_{x'} \tag{A9}$$

$$B = \int_0^{t_0} dt \int_{S_{1,0}} \frac{E_{x''}(x,t_0-t) \frac{\partial^2}{\partial n \partial n''} G_0(x,x'',t)}{Q(x'',t_0)} dS_x \tag{A10}$$

Equation (43) giving

$$A + B = 1 \tag{A11}$$

$U(E_i/E_u)$ and $L(E_i/E_j)$ are respectively the upper bound and the lower bound of the ratio

$E_i(x,t)/E_j(x,t)$ for x on $S_{1,0}$ and $0 \leq t \leq t_0$.

We now proceed to show that both A and B are non-negative, a result necessary for the assertion (A7).

Using the symmetry property of Green's functions

$$G_i(x,x',t) = G_i(x',x,t)$$

we can rewrite A in the form

$$A = \frac{\int_{\Omega_0} - \frac{\partial}{\partial n'} G_0(x'',x',t_0)dV_{x'}}{Q_2(x'',t_0)} = \frac{Q_0(x'',t_0)}{Q_2(x'',t_0)}$$

Taking (A4a) into account, we obtain

$$A \geq 0 \tag{A9a}$$

or, taking (A4b) into account:

$$A>0 \quad \text{for} \quad t_0<\infty \tag{A9b}$$

Now consider the expression (A10) of B. Both $E_{x''}(x,t_0-t)$ and $Q(x'',t_0)$ are non-negative (Equation A3a and A4a).

The remaining term will be shown to be also non-negative.

Indeed, it can be rewritten as

$$B_1 = \frac{\partial^2}{\partial n \partial n''} G_0(x,x'',t) = \frac{-\partial}{\partial n''} \left[\frac{-\partial}{\partial n} G_0(x,x'',t)\right]$$

or, using the boundary condition (6)

$$B_1 = \frac{-\partial}{\partial n''} \left[\frac{1}{\alpha(x)} G(x,x'',t)\right] = \frac{1}{\alpha(x)} \frac{-\partial}{\partial n''} G(x,x'',t)$$

Using the property of symmetry

$$B_1 = \frac{1}{\alpha(x)} \frac{-\partial}{\partial n''} G(x'',x,t)$$

Involving Equation (6) again, we obtain:

$$B_1 = \frac{1}{\alpha(x)} \frac{1}{\alpha(x'')} G(x'',x,t) \geq 0$$

All terms of the integrand of B (Equation 10) being non-negative, we have

$$B \geq 0 \tag{A10a}$$

In order to determine the bounds of E_i/E_j, we turn to consider Equation (36) which we rewrite in the form

$$G_j(x'',x',t_0) = G_i(x',x'',t_0)$$

$$+ \int_0^{t_0} dt \int_{S_{1,i}} G_j(x,x',t_0-t) \frac{-\partial}{\partial n} G_i(x,x'',t)dS_x \tag{A12}$$

where $\Omega_i \subset \Omega_j$. (A13)

Integrating Equation (A12) over $x' \varepsilon \Omega_j$, we obtain

$$E_j(x'',t_0) = E_i(x'',t_0)$$

$$+ \int_0^{t_0} dt \int_{S_{1,i}} E_j(x,t_0-t) \frac{-\partial}{\partial n} G_i(x,x'',t)dS_x \tag{A14}$$

which leads to the inequality

$$E_i(x,t) \leq E_j(x,t) \tag{A15}$$

provided (A13) is true.

Let i=1 and j=2. As $\Omega_1 \subset \Omega_2$, (A15) gives

$$E_1(x,t) \leq E_2(x,t)$$

or

$$\mathbf{U}(E_1/E_2) = 1. \tag{A16}$$

Substituting the above expressions into (A7) and taking (A11) into account, we obtain

$$Q_1(x'',t_0)/Q(x'',t_0) \leq 1 \tag{A17}$$

Let us write the inequality (A4a) for i=3:

$$E_3(x,t) \geq 0$$

giving

$$L(E_3/E_2) = 0 \qquad \text{(A18)}$$

Substituting that equation into (A8) we obtain

$$Q_3(x",t_0)/Q(x",t_0) \geq A \qquad \text{(A19)}$$

Finally, Equation (A17) and (A19) imply

$$\frac{Q_1(x",t_0)}{Q_3(x",t_0)} \leq \frac{1}{A} \qquad \text{(A20)}$$

As $A>0$ for $t_0<\infty$ (see Equation A9b), Equation (A20) implies:

$$\frac{Q_1(x",t_0)}{Q_3(x",t_0)} < \infty \qquad \text{(A21)}$$

Substituting Equation (A3) for i=1 and 3 into (A21) we obtain (A1) Q.E.D.

The current proof required only tangency of surfaces Σ_1 and Σ_3. The introduction of a very special surface Σ_2, such that $\Omega_1 C \Omega_2$ and $\Omega_3 C \Omega_2$, was for construction of the proof only. In the rest of the text, the restrictions on Σ_2 are only those imposed here on Σ_3.

APPENDIX B

Expressions for $H^3(t,t_0)$

$H^3(t,t_0)$ is defined by Equation (74) of Section VI.2.2. Starting from the early time expansion Equation (109), we derive*

$$H^3(t,t_0) = -\mathrm{erf}(u_2) + \sum_{m=1}^{\infty} \left\{ 2\sqrt{\frac{t_0}{t}}\, \mathrm{erf}(u)\, e^{-\frac{(2m-1)^2}{4t}} - e^{-\frac{m^2}{t_0}} \left[\mathrm{erf}(u_1+u_2) - \mathrm{erf}(u_1-u_2) \right] \right\} \tag{B1}$$

where

$$u_1 = \sqrt{\frac{t_0-t}{t\, t_0}} \quad ; \quad u_2 = \frac{1}{2}\sqrt{\frac{t_0}{t(t_0-t)}} \quad ; \quad u = \frac{1}{2\sqrt{t_0-t}}$$

Starting from the eigenvalue expansion Equation (108):

$$H^3(t,t_0) = 2\sqrt{\pi t_0} \sum_{m=1}^{\infty} \left[\mathrm{erf}(u)(-1)^m e^{-m^2\pi^2 t} - e^{-m^2\pi^2 t_0} R_m \right] \tag{B2}$$

where

$$u = 1/2\sqrt{t_0-t}$$

and

$$R_m = \frac{1}{2}\left[\mathrm{erf}\left(u + i\,\frac{m\pi}{u}\right) + \mathrm{erf}\left(u - i\,\frac{m\pi}{u}\right) \right] \tag{B3}$$

or

$$R_m = \mathrm{erf}(u) + \frac{e^{-u^2}}{2\pi u}\left[1-(-1)^m\right] + \frac{4u}{\pi} e^{-u^2} \sum_{n=1}^{\infty} \frac{e^{-n^2/4}}{u^2+4n^2} \left[1-(-1)^n \operatorname{Cosh} \frac{nm\pi}{2u} \right] \tag{B4}$$

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*The derivations are given in MAGI's internal memorandum P-7133, Sept. 13, 1976.

X. REFERENCES

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2. H. S. Carslow and J. C. Jaeger, "Conductor of Heat in Solids", Second Edition, Oxford University Press, London (1959).